I YEAR - I SEMESTER
COURSE CODE: 7BCH1C1

CORE COURSE – I - FUNDAMENTALS OF CHEMISTRY

Unit I Atomic and molecular composition of matter:

1.1. Atom – constituents of an atom. Elementary particles and composite particles (hadrons). Atomic Structure. Bohr's theory and its limitations, dual behaviour of matter and radiation, de Broglie's relation, Heisenberg Uncertainty principle. Atomic spectrum of hydrogen. Zeemann effect. Molecules – molecular weight – mole – Avogadro number – calculating number of moles.

1.2. **Quantum mechanics:** Fundamental postulates of quantum mechanics. Time independent Schrodinger equation and meaning of various terms in it. Significance of ψ and ψ^2. Schrödinger equation for hydrogen atom. Radial and angular parts of the wave functions (atomic orbitals) and their variations for 1s, 2s, 2p, 3s, 3p and 3d orbitals (Only graphical representation). Radial and angular nodes and their significance. Radial distribution functions and the concept of the most probable distance with special reference to 1s and 2s atomic orbitals.

1.3. Quantum numbers – principal – orbital – angular momentum quantum numbers (n, l and m). Significances of quantum numbers. Shapes of s, p and d atomic orbitals, nodal planes. Discovery of spin – spin quantum number (s). Rules for filling electrons in various orbitals, Electronic configurations of the atoms. Relative energies of atomic orbitals – anomalous electronic configurations.

Unit II Periodic table:

2.1. **Periodicity of Elements:** Modern periodic law. Structure of modern periodic table (long form of periodic table). Classification of elements as s, p, d, f block elements.

2.2. **Periodic variation of properties:** Detailed discussion on the variation various fundamental properties of the elements. Effective nuclear charge – shielding or screening effect and Slater rules. Atomic radii (van der Waals) and ionic radii. Ionization enthalpy, successive ionization enthalpies and factors affecting ionization energy and applications of ionization enthalpy. Electron gain enthalpy, trends of electron gain enthalpy. Electronegativity, Pauling's/ Mulliken's/ Allred Rachow's/ and Mulliken-Jaffe's electronegativity scales. Variation of metallic character in periodic table.

2.3. **Comparison of different groups and periods:** anomalies between first and second rows. Diagonal relationships. Participation of d – orbital in compound formation. Periodic anomalies of the non-metals and posttransition metals.

Unit III

3.1. Sources of organic compounds.

3.2. Naming of organic compounds with single or more number of functional groups in trivial and IUPAC systems.

3.3. Molecular weight determination of organic acids and bases by silver salt and platinichloride methods. Problems arriving empirical and molecular formula using percentage composition of elements and molecular weight.

3.4.Structural formula – Shapes of organic molecules. sp3, sp2 and sp hybridization in organic compounds with suitable examples.

3.5.Classification of organic compounds as aliphatic, aromatic, alicyclic and hetero cyclic compounds.

3.6.Steric and electromeric effects. Inductive effect, +I and –I effects, resonance effects (delocalized chemical bonding), rules for resonance, resonance stabilization energy, hyperconjugation. Explanation with suitable examples for each.

Unit IV Physical properties and chemical constitution:

4.1 Classification of physical properties of materials as additive properties, constitutive properties, additive constitutive properties and colligative properties with suitable examples. Vector and scalar properties with suitable examples. Extensive and intensive properties.

4.2 Dipole moment, calculation of dipole moment and bond length. Bond moment and dipole moment. Calculating percentage of ionic character from dipole moment and electronegativity differences.

4.3 Magnetic properties, para, dia, ferro antiferro and ferri magnetism. Curie temperature (TC). Magnetic susceptibility, Determination of magnetic susceptibility, spin only magnetic moment and its relationship to number of unpaired electrons.

4.4 Molar volume, surface tension and parachor. Atomic and structural parachors and their uses to fix the exact structure.

Unit V Introduction to computers:

5.1. **Basics:** Types of computer – different components o a computer – constants – variables – bits and bytes. Binary number system – representation of integers – conversion of a decimal to binary and vice- versa. Other number systems and their mutual conversion.

5.2. Programming – algorithm – flow charts , operating systems. Expressions, hierarchy of operations, inbuilt functions. Elements of the BASIC language. BASIC keywords and commands. Logical and relative operators. Compiled versus interpreted languages. Debugging. Simple programs using these concepts for calculating the rate constants, velocity of gaseous molecules and molar concentration, normality of a solution, matrix addition, matrix Multiplication and statistical analysis.

5.3. List of computer software and their uses in chemistry.

Text Books:

1. Inorganic chemistry – R.D. Madhan
2. Advanced inorganic chemistry – Sathyaprakash
3. Inorganic Chemistry – J.D. Lee
4. Organic chemistry – PL. Soni
5. Organic Chemistry – Sharma
6. Organic Chemistry – Morrison & Boyd
7. Organic Chemistry – I.L. Finar (Vol. I & II)
8. Advanced Physical Chemistry –Puri,Sharma & Pathania.
9. Physical Chemistry – G. W. Castellan 7th edition
10. Physical Chemistry – S. Glasstone

Fundamental Concepts in Chemistry.

IBCHIC1

Unit - I

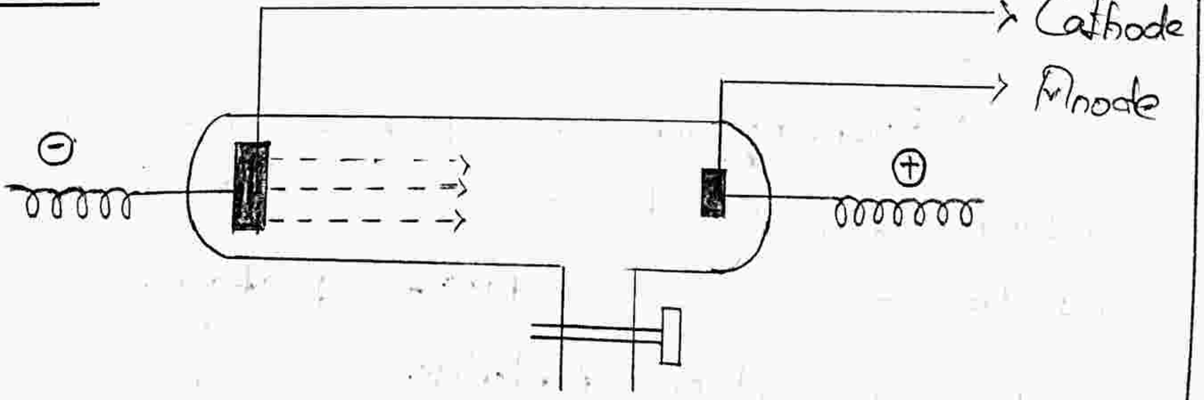
ATOMIC STRUCTURE :-

ATOM - Constituent Of an atom :-

The idea of atom was first given by Hindu & Greek philosophers. On the basis of law of chemical combination, John Dalton gave the atomic theory.

∴ Matter is made up of very small indivisible particles called atom. But it is not indivisible. It has a complex structure & made up of electron, proton & Neutron. They are called Sub-atomic particles.

Electron :-



When a gas at low pr (0.01mm) was Subjected to a high electric potential (10000 Volt) a stream of rays were emitted from cathode. These cathode rays contain negatively charged particles called electrons.

Proton:

Goldstein discovered protons. He passed high Voltage through a gas at low pressure in a discharge tube provided with a perforated cathode.

cathode rays & luminous rays passing backward through the minute holes of the cathode. These are called anode rays (or) canal rays (or) positive rays.

Neutron:

At. No. of H $^1H \Rightarrow$ 1 proton

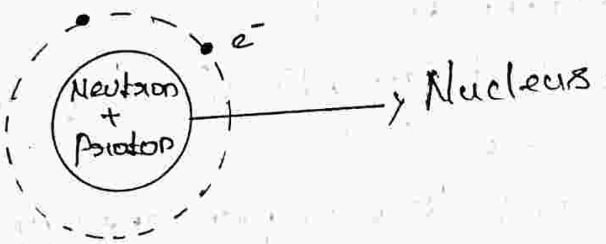
$^2He \Rightarrow$ 2 proton.

Thus He is twice heavy as H. But it is 4 times wt. of H_2.

∴ Rutherford predicted in 1920 some neutral particles having mass equal to protons must be present in the nuclei of atoms. This was later confirmed by chadwick.

He discovered these neutral particles in 1932 by bombarding light elements like Li, Be, B, etc. with α particle. He called the neutrons.

$_4Be^9 + {}_2He^4 \rightarrow {}_6C^{12} + {}_0n^1$



neutron + proton ⟹ nucleons.

	charge	Mass	Symbol
Proton	+1	1	$_1p^1$
Newtron	0	1	$_0n^1$
Electron	−1	0	$_{-1}e$

Bohr Model Of Atomic Structure:

Bohr's atom model is based on Quantum Theory.

Postulates Of Bohr's theory:

* Electrons revolve around the nucleus in certain permitted circular orbits called stationary states (or) energy levels.

* The angular momentum of the electron moving in the stationary orbit is an integral multiple of h/2π Mathematically:

$$\boxed{mvr = n\frac{h}{2\pi}}$$

Where 'n' is known as principle Quantum number (1, 2, 3, 4, etc...)

This is called Quantisation of angular momentum.

* As long as the electron revolves in the stationary orbit, it does not lose (or) gain energy.

* The electron will absorb energy in packets (or) quanta & goes to a higher energy orbit. Under such condition the atom is said to be in the excited state

* The electron come back from the excited state to the ground state in one (or) more jumps by emitted energy.

* The energy difference between the two orbits is given by $\boxed{E_2 - E_1 = \Delta E = h\nu.}$

where,

E_2 - Energy of higher orbit,

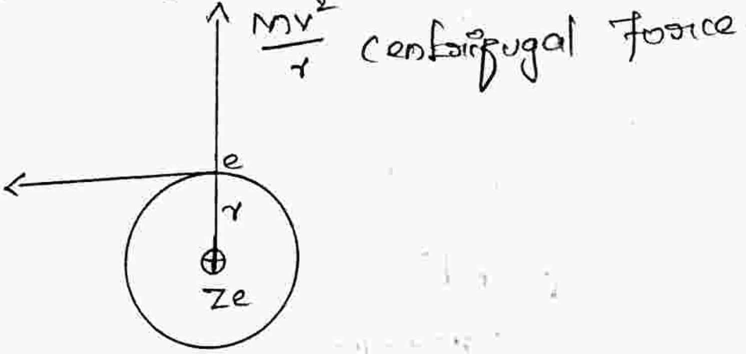
E_1 - Energy of lower orbit,

ν - frequency of radiation.

* Each line observed in the atomic spectrum is due to the energy emitted when an electron jumps from higher orbit to the lower orbit.

Derivation of Bohr's Radius:

Consider an electron of charge 'e' revolving round a nucleus of charge 'Ze' (where Z is the atomic number & e is the charge of a proton). Let 'm' be the mass of the electron & 'r' be the radius of the orbital.



The electrostatic force of the attraction between the nucleus and the electron $\Big\} = \frac{Ze \cdot e}{r^2}$

$$= \frac{Ze^2}{r^2}$$

The centrifugal force acting on the electron $\Big\} = \frac{mv^2}{r}$

To keep the electron in the stationary orbit, the two forces balances each other.

$$\frac{mv^2}{r} = \frac{Ze^2}{r^2}$$

$$v^2 = \frac{Ze^2}{mr} \quad \text{—} ①$$

According to Bohr's theory the angular momentum.

$$mvr = n\frac{h}{2\pi}$$

Squaring on both sides, we get

$$m^2v^2r^2 = \frac{n^2h^2}{4\pi^2}$$

$$v^2 = \frac{n^2h^2}{4\pi^2m^2r^2} \quad \text{———} ②$$

compare ① & ②

$$\frac{Ze^2}{mr} = \frac{n^2h^2}{4\pi^2m^2r^2}$$

$$r = \frac{n^2h^2}{4\pi^2Ze^2m}$$

For H atom, $Z = 1$

$$\therefore r = \frac{n^2h^2}{4\pi^2me^2}$$

In S.I unit, $r = \dfrac{n^2h^2(4\pi\varepsilon_0)}{4\pi^2me^2}$

$$\boxed{r = \frac{n^2h^2\varepsilon_0}{\pi me^2}}$$

Radius of Bohr's first orbit ($n=1$) for H atom is

$$r_1 = \frac{1^2 \times (6.626\times10^{-34})^2 \times 8.85\times10^{-12}}{3.14 \times 9.1\times10^{-34} \times (1.602\times10^{-19})^2}$$

$$r_1 = 0.53\,A^\circ$$

The radius of 2nd to 5th orbits are.

$r_2 = 2^2 \times 0.53 = 2.12A^\circ$ $\qquad$ $r_3 = 3^2 \times 0.53 = 4.77A^\circ$

$r_4 = 4^2 \times 0.53 = 8.48A^\circ$ $\qquad$ $r_4 = 4^2 \times 0.53 = 13.25A^\circ$

Derivation of energy of revolving electron:-

Total energy of electron in any orbit is the sum of potential & kinetic energies.

Potential energy of an electron in an orbit is given by the work done in taking the electron from infinite distance to the orbit.

$$P.E = -\frac{Ze^2}{r}$$

Kinetric Energy, $(K.E) = \frac{1}{2}mv^2.$

$$= \frac{1}{2} m \frac{Ze^2}{mr} \left(\text{since } v^2 = \frac{Ze^2}{mr}\right)$$

$$K.E = \frac{1}{2}\frac{Ze^2}{r}$$

Total Energy, $E = P.E + K.E.$

$$= -\frac{Ze^2}{r} + \frac{1}{2}\frac{Ze^2}{r}$$

$$E = -\frac{1}{2}\frac{Ze^2}{r} \text{ —— } ①$$

Subs the value of $r = \frac{n^2h^2}{4\pi^2 Ze^2 m}$ in eqn ①

$$E = -\frac{1}{2}\frac{Ze^2 4\pi^2 Ze^2 m}{n^2h^2}$$

$$E = -\frac{2\pi^2 Z^2 m e^4}{n^2h^2}$$

For H atom, $Z = 1$

$$\therefore E = -\frac{2\pi^2 m e^4}{n^2h^2}$$

In S.I Unit, $E = -\frac{1}{(4\pi\epsilon_0)^2} \times \frac{2\pi^2 m e^4}{n^2 h^2}$

$$\boxed{\therefore E = -\frac{1}{n^2}\left(\frac{me^4}{8\epsilon_0^2 h^2}\right)}$$

Energy of the first & second orbits of hydrogen atoms are

$$E_1 = -\frac{1}{1^2}\left[\frac{9.1\times10^{-31}\times(1.602\times10^{-19})^4}{8\times(8.85\times10^{-12})^2\times(6.626\times10^{-34})^2}\right]$$

$$E_1 = -2.178\times10^{-18} J$$

$$E_2 = -0.5445\times10^{-18} J$$

$$E_3 = -0.242\times10^{-18} J.$$

Thus the orbits K, L, M are in the order of increasing energy.

Limitations Of Bohr's Theory :-

* Bohr's Theory is not successfull in explaining the spectra of atoms containing more than one electron (He, Li, Be, ...).

* Bohr's theory failed to explain the fine structure of spectral lines.

* Bohr's atomic Model couldn't explaining the splitting of spectral lines in the external electric & Magnetic fields (i.e. Stark & Zeeman effect respectively)

* Bohr's theory failed to consider the wave property of electron.

* Bohr's theory doesn't take into account the spin of nucleus.

* Bohr's theory doesn't tell anything about the distribution & arrangement of electrons in an atom.

* Bohr's theory assumes that electrons move in definite orbits. This is against Heisenberg's uncertainty principle.

Dual Nature of Matter: de-Broglie's concept.

In 1905, Einstein suggested that light has a dual character: the particle & the wave nature. properties like diffraction & interference support the wave nature of light. photoelectric effect & compton effect support the particle nature of light.

In 1924, Louis de Broglie suggested that Matter also has dual character: the particle & the Wave nature.

In Bohr's theory electron is treated as a Particle. But the de-Broglie's theory suggested that electron has a dual character. both as a particle & Wave.

According to de-Broglie, the Wavelength (λ) of a moving particle of Mass & moving with a Velocity (v) is given by.

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

Where h is planck's constant. This equation is called de-Broglie's Wave equation & λ is called de-Broglie's Wavelength.

Significance Of de Broglie's Concept:

* The Wave character of small object (in motion) has considerable significance, since its wavelength is easily observed in electronic spectrum.

* The Wavelength of large object (in motion) has no practical significance since the Wavelenth is too small to be observed & hence cannot be Measured.

de-Broglie's Equation:

de-Broglie derived an expression relating Momentum & Wavelenth of a particle in motion.

Consider a photon of energy (E) with frequency (ν) & wavelength (λ), then

$$E = h\nu = \frac{hc}{\lambda} \quad \text{——} ①$$

From Einsteins eqn,

$$E = mc^2 \text{——} ②$$

Compare eqn ① & ②

$$\frac{hc}{\lambda} = mc^2$$

$$\lambda = \frac{h}{mc} \quad \text{——} ③$$

$$\boxed{\lambda = \frac{h}{mv}} \text{——} ④$$ [where v- velocity of electron]

$\therefore mv = p$, the momentum of the particle.

$$\boxed{\lambda = \frac{h}{p}} \quad — ⑤$$

The eqn ④ & ⑤ are called de-Broglie's Equation.

Heisenberg Uncertainty Principle:

According to Heisenberg Uncertainty principle "It is not possible to determine exactly both the position & the momentum (velocity) of a small moving particle.

He showed that the product of uncertainties in position (Δx) & Momentum (Δp) is related to planck's constant (h) as.

$$\Delta x . \Delta p \geq \frac{h}{4\pi} \quad — ①$$

Where Δx - Uncertainty in position
Δp - Uncertainty in Momentum
h - planck's constant.

(The sign $\geq$ means that the product of Δx & Δp is equal (or) greater than $\frac{h}{4\pi}$ but never less than $\frac{h}{4\pi}$)

$\therefore$ The eqn be $\Delta x . \Delta p = \frac{h}{4\pi}$ — ②

Since $\Delta p = m \Delta v$ (m - Mass of the particle & Δv - uncertainty in velocity)

Eqn ② becomes

$$\boxed{\Delta x . m . \Delta v = \frac{h}{4\pi}}$$

An attempt to locate the exact position of the electron will make uncertainty in its momentum. Visible light cannot be used to locate the exact position of electron as the Wavelength is higher. If we use x-rays to locate the electrons, it gets accelerated due to compton effect & produces uncertainty in the momentum.

Similarly an attempt to determine the exact momentum of the electron will introduce uncertainty in its position.

This uncertainty arises not due to the defect in the experiment technique, but it is the fundamental principle of nature itself.

Significance:-

* The product of uncertainty in position & Momentum depends upon the mass of the particle. The uncertainty will be more significant for a small particle like electron than a bigger particle like a bell.

* It is a proof for dual nature of electron

* If the position of the particle is determined more (or) less exactly then Δp would be large. i.e. Uncertainty in momentum will be lose.

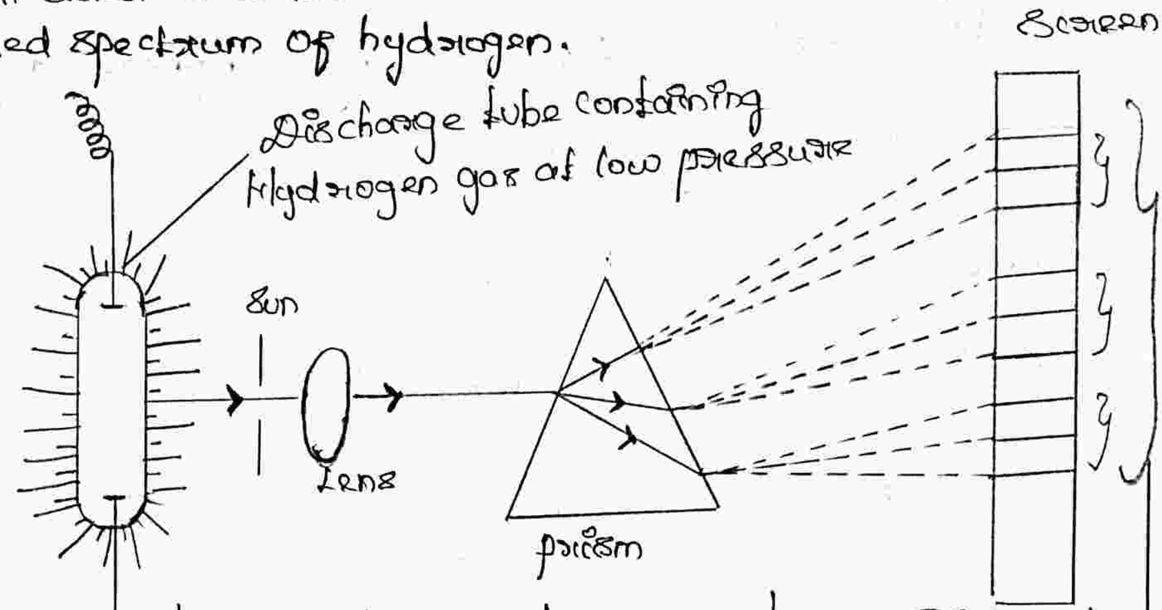
Hydrogen Spectrum:-

This spectrum, like the atomic spectrum ~~like~~ given by other elements, is also known by other names like emission spectrum (or) atomic emission spectrum of hydrogen.

How is hydrogen Spectrum Obtained?

When an electric discharge is passed through hydrogen gas filled in a discharge tube at very low

~~temperature~~ pressure, a bluish light is emitted from the discharge tube. When the ray of this bluish emitted light is passed through a prism. a discontinuous line spectrum consisting of several isolated sharp lines with dark area in between is obtained. such a spectrum is called spectrum of hydrogen.



Line spectrum of hydrogen atom observed on passing light emitted from a discharge tube (containing) (Hydrogen) through a prism.

When an electric discharge is passed through hydrogen, the molecules of hydrogen break into atom. These absorb energy from the electric spark & get excited. The excited atoms give the extra energy in the form of emitted light (bluish light). When this emitted light is allowed to pass through a prism line spectrum of hydrogen is obtained. This spectrum is also called line emission spectrum.

Classification of spectral lines in Hydrogen Spectrum:

All these spectral lines can be classified into 5 groups called spectral series which are named after their discoverers as shown below:

Spectral series	Discovered by	Appeared in
(i) Lyman series	Lyman	Ultraviolet region.
(ii) Balmer series	Balmer	Visible region
(iii) Paschen series	Paschen	Infra-red region
(iv) Brackett series	Brackett	Infra-red region
(v) Pfund series	Pfund	Infra-red region

Zeeman Effect:-

If a substance which gave a line emission spectrum is placed in a magnetic field, the lines of the spectrum get split up into a no. of closely spaced lines. This phenomenon is known as Zeeman Effect.

Hadron:

A hadron is a composite particle made of quarks held together by the strong force in a similar way as molecules are held together by the electromagnetic force. Of the hadrons, protons are stable, & neutrons bound with atomic nuclei are stable. other hadrons are unstable under ordinary condition.

Molecules:

A Molecule is an electrically Neutral group of two (or) more atoms held together by chemical bond.

A molecule may be homonuclear, that is it consists of atoms of one chemical element.

eg :- O_2

It may be heteronuclear, a chemical compound consists of more than one element.

eg :- H_2O.

Molecular Mass (or) Molecular Weight :-

It is calculated as the sum of the atomic Weights of each constituent element multiplied by the number of atoms of that element in the Molecular formula.

The molecular mass of small to medium size molecules, measured by mass spectrometry, determines stoichiometry. For large Molecules, such as proteins, Methods based on Viscosity, & light-scattering can be used to determine molecular mass when crystallographic data are not available.

The molecular weight of Methane. The Molecular formula is CH_4 can be shown below.

	Atomic Mass	Total Mass
C	12.011	12.011
H	1.00794	4.03176
CH_4		16.043

Glucose ($C_6H_{12}O_6$)

6 - carbon atoms (Atomic Mass of carbon is 12.011)
12 - Hydrogen atom (Atomic Mass of 'H' is 1.008)
6 - oxygen atom (Atomic Mass of 'O' is 15.999)

Molecular Weight = $(6 \times 12.011) + (12 \times 1.008) + (6 \times 15.999)$
$= 72.066 + 12.096 + 95.994$
$= 180.156$ //.

Avogadro's Number (N_A).

The number of atoms in a 12g sample value [illegible] of carbon-12 is called Avogadro's Number.

Recent measurements of this Number give the Value 6.0221367×10^{23}, which is 6.023×10^{23}.

A mole of a substance contains Avogado number of molecules. A dozen eggs equals 12 eggs A gross of pencils equals 144 pencils & a mole of ethanol equals 6.023×10^{23} ethane molecules.

Significance :-

The molecular Mass Of SO_2 is $64 g mol^{-1}$. 64g of SO_2 contain 6.023×10^{23} molecules of SO_2. $2.24 \times 10^{-2} m^3$ of SO_2 at S.T.P. contain 6.023×10^{23} molecules of SO_2.

Similarly the molecular mass of CO_2 is $44 g mol^{-1}$ 44g of CO_2 contains 6.023×10^{23} molecule of CO_2. $2.24 \times 10^{-2} m^3$ of CO_2 at S.T.P contains 6.023×10^{23} molecules of CO_2.

Mole Concept :-

While carrying out reaction we are often interested in knowing the number Of Atoms (or) Molecules of different reactions in a definite ratio

eg :- consider the following reactions are

$$2H_2 + O_2 \longrightarrow 2H_2O.$$

In this reaction one molecule of oxygen reacts with two Molecules of hydrogen. so, it would be desirable to take the Molecules of H_2 & oxygen in the ratio 2:1, so, that the Reactions are completely Consumed during the reaction. But atoms & Molecules are so small in size that is not possible to count them individually.

In order to overcome these difficulties, the concept of mole was introduced. Accordingly to this concept number of particles of the substance is related to the mass of the substance.

Definition:-

The mole may be defined as the amount of the substance that contains as many specified, elementary particles as the number of atoms in 12g of carbon-12 isotope.

(i.e) one Mole of an atom consists of Avogadro Number of particles.

One Mole = 6.023×10^{23} particles.

One Mole of oxygen = 6.023×10^{23} Oxygen

one Mole of ethanol = 6.023×10^{23} ethanol.

In Using the term Mole for ionic substances, We mean the number of formula units of the substance. For example, a Mole of Sodium carbonate (Na_2CO_3) is a quantity containing 6.023×10^{23} Na_2CO_3 units. But each formula unit of Na_2CO_3 contains $2 \times 6.023 \times 10^{23}$ Na^+ ions & one CO_3^{2-} ions & $1 \times 6.023 \times 10^{23}$ CO_3^{2-} ions.

When Using the term Mole, it is important to specify the formula of the unit to avoid any misunderstanding.

eg) A mole of oxygen atom contains 6.023×10^{23} Oxygen atoms. A mole of oxygen ~~atom~~ Molecule contains 6.023×10^{23} O_2 molecules (ie) $2 \times 6.023 \times 10^{23}$ oxygen.

Calculating the Number Of Moles :-

To find the Mass of One Mole of substance. There are two important things to know.

=> How Much does a given number of Moles Of a substance Weight?

=> How Many moles of a given formula unit does a given mass of substance contain.

Both of them can be known by using dimensional analysis.

To convert Mole of ethanol to grams of ethanol. We simply convert the conversion factor (46.1g C_2H_5OH / 1mole C_2H_5OH).

Again, Suppose you are going to prepare acetic acid from 10.0g of ethanol (C_2H_5OH). How many moles of C_2H_5OH is this? you convert 10.0g C_2H_5OH to moles C_2H_5OH by multiplying by the appropriate conversion factor.

$$10.0g\ C_2H_5OH \times \frac{1mol\ C_2H_5OH}{46.1g\ C_2H_5OH} = 0.217\ Mol\ C_2H_5OH$$

Quantum Mechanics (Wave Mechanics) :-

classical Mechanics is obeyed by "Macroscopic particles" such as planets & rigid bodies. However, since the Microscopic particles such as electrons, protons, atoms & Molecules show Wave particle duality, they do not obey Newtonian dynamics. They, However, obey Quantum Mechanics (or Wave Mechanics) a key feature of which is the Quantization of energy & angular Momentum.

Postulates Of Quantum Mechanics:-

First postulate:

The physical state of a system at time 't' is described by Wavefunction $\psi_{(x,t)}$.

Second Postulate:

The Wavefunction $\psi(x,t)$ & its first & second derivatives $\partial\psi(x,t)/\partial x$ & $\partial^2\psi(x,t)/\partial x^2$ are continuous, finite & single valued for all values of x. Also, the wavefunction $\psi(x,t)$ is normalized.

i.e, $\boxed{\int_{-\infty}^{\infty} \psi^*(x,t)\,\psi(x,t)\,dx = 1}$

When

ψ^* is the complex conjugate of ψ.

Third Postulate:-

A physically observed Quantity can be represented by a Hermitian operator. An operator $\hat{A}$ is said to be Hermitian if it satisfies the following condition:

$$\boxed{\int \psi_i^* \hat{A} \psi_j \, dx = \int \psi_j (\hat{A}\psi_i)^* dx.}$$

Where,

ψ_i & ψ_j are the Wavefunctions representing the physical state of the Quantum System, such as a particle, an atom (or) a Molecule.

Fourth postulate:

The allowed Values of an observable A are the eigenvalues, ai, in the operator equation.

$\hat{A}\psi_i = a_i\psi_i$ is known as eigenvalue equation. Here $\hat{A}$ is the operator for the observable (physical Quantity). & ψi is an eigenfunction of $\hat{A}$ with eigenvalue ai.

Fifth Postulate:

The average Value (or the expectation Value). <A> of an observable A corresponding to the operator $\hat{A}$, is obtained from the relation.

$$\langle A \rangle = \int_{-\infty}^{\infty} \psi^* \hat{x} \psi \, dx.$$

Sixth postulate:

The Quantum Mechanical operators corresponding to the observales are constructed by writing the classical expression in terms of the Variables & converting the expressions to the operators.

Seventh Postulate:

The Wave function ψ(x,t) is a solution of the time dependent schordinger equation.

$$\hat{H}\psi(x,t) = i\hbar \frac{\partial \psi(x,t)}{\partial t}$$

Where, $\hat{H}$ is the Hamiltonian operator of the System.

Time Independent Schrodinger Wave equation.

In Schrodinger Wave model of an atom, the discrete energy level (or) orbits proposed by Bohr are replaced by mathematical functions, ψ, which are related to the probability of finding electrons at various places around the nucleus.

Consider a simple wave motion as that of the vibration of a streched string. Let y be the amplitude of the vibration at any point whose co-ordinate ais 'x' at time 't'. This equation is.

$$\frac{\partial^2 y}{\partial x^2} = \frac{1}{u^2}\left(\frac{\partial^2 y}{\partial t^2}\right) \text{ --- ①}$$

u, - velocity   i.e, the amplitude y depends upon
x,t - Variable   two variable x & t.

$$y = f(x)\cdot g(t) \text{ --- ②}$$

where

f(x) is a function of the coordinate x only

& g(t) is a function of the time 't' only.

Then, $g(t) = A\sin(2\pi\nu t)$ --- ③

ν - vibrating frequency, A - constant

so, $Y = f(x)A\sin(2\pi\nu t)$ --- ④

Hence, $\frac{\partial^2 Y}{dt^2} = f(x)4\pi^2\nu^2 A\sin(2\pi\nu^2 t)$ --- ⑤

Similarly $\frac{\partial^2 y}{dt^2} = -4\pi^2\nu^2 f(x)\,g(t)$ --- ⑥

$$\frac{\partial^2 y}{dx^2} = \frac{\partial^2 f(x)}{\partial x^2}g(t) \text{ --- ⑦}$$

combaining eqn ⑦, ⑥ & ④, we get.

$$\frac{\partial^2 f(x)}{\partial x^2} = \frac{-4\pi^2\nu^2}{\nu^2} f(x) \quad \text{———} ⑧$$

The frequency of the vibrations ν is related to the velocity (u) by the expression $u = \nu\lambda$, λ is corresponding to the length

$$\frac{\partial^2 f(x)}{\partial x^2} = \frac{-4\pi^2}{\lambda^2} f(x)$$

We may extended it to 3 dimensions represented by the coordinates x, y & z. i.e (x, y, z)

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} = \frac{-4\pi^2}{\lambda^2} ~~for~~ \psi \quad \text{———} ⑨$$

De-Broglie's relationship $\lambda = \frac{h}{mu}$

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} = \frac{-4\pi^2 m^2 u^2}{h^2} \psi \quad \text{———} ⑩$$

∴ m - mass, u - velocity.

Kinetic energy (K.E) $= \frac{1}{2}mu^2 = E - V$ (or)

$$mu^2 = 2(E - V) \quad \text{———} ⑪$$

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{8\pi^2 m(E - V)}{h^2} \psi = 0 \quad \text{———} ⑫$$

It is known as Schrodinger Wave equation.

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V\right] = E\psi \quad \text{———} ⑬ \quad \left[\because \hbar = \frac{h}{2\pi}\right]$$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V\right]\cdot\psi = E\psi \quad \text{———} ⑭$$

∇^2 is the Laplacian operator.

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Hamiltonian Operator, $\hat{H} = \frac{-\hbar^2}{2m}\nabla^2 + V$

The Time Independent schrodinger Wave eqn (14) becomes.

$$\hat{H}\psi = E\psi \quad \text{— (15)}$$

The schrodinger Wave eqn can have several solutions not all of which corresponded to any physical (or) chemical ~~reaction~~ reality, such solutions (or) Wave functions are therefore not accepted

The acceptable wave functions must satisfy the following conditions.

⇒ The wave function ψ is single valued i.e, for each value of the variable x, y, z there is only one value of ψ. Suppose one of the variables is an angle θ. Then, single-valuedness of ψ requires that.

$$\psi(\theta) = \psi(\theta + 2n\pi) \quad [\therefore n \text{ is an integer}]$$

⇒ The Wave function ψ & its first derivative with respect to the variables must be continuous. (i.e) there must not be any sudden change in ψ when its variables are changed.

⇒ For bound states, ψ must vanish at infinity. If ψ is complex function. Then $\psi^*\psi$ must vanish at infinity (ψ^* is the complex conjugate of ψ).

Satisfying the above conditions, the schrodinger eqn yields significant solutions for certain definite values of the total energy E. These values are called Eigen values.

$\hat{H}\psi_n = E_n \psi_n$ $(n = 1, 2, 3, \ldots\ldots)$

Where, n - Quantum Number

ψ_n - Eigen Function

E_n - Eigen Value.

=> The eigen functions are said to form an orthonormal set if

$$\int \psi_n^* \psi_m \, dx = \begin{cases} 0, & n \neq m \\ 1 & n = m \end{cases} = \delta_m$$ (called the Kronecker delta)

Significan of Schrodinger Wave Function:-

* It is a second order differential equation which relates the wave function ψ with energy E

* This equation can be solved only for certain integral values of Eigen Values. The corresponding functions are called Eigen Functions.

* For Eigen functions, ψ must be finite, single valued & continuous.

* Solutions of Schrodinger wave equation involves certain constants called Quantum numbers 'n', 'l' & m.

Applications:-

* It introduces the term atomic orbital.

* It is used to derive the expression for energy of an electron in hydrogen atom.

* It is used to calculate the energy & wave function of particles in one dimensional & three dimensional Box.

Nature of Wave function ψ

* ψ represents the amplitude of spherical wave function. The wave function ψ may be considered as an amplitude function expressed interms of 3 co-ordinates x, y & z

* ψ can have positive (or) Negative values depending on the values of the co-ordinate

* The magnitude of ψ will give the amplitude of electron wave

* When we solve the Schrodinger wave equation, we find some regions of space in which ψ is positive & other regions in which ψ is negative. But the probability must be always positive & cannot be negative. Therefore we have to use ψ^2 instead of ψ.

Significance of ψ^2

* ψ^2 is a probability density function.

* It gives the probability of finding an electron within small space around the nucleus.

* ψ^2 may be large, small (or) zero but it can't be imaginary

* The probability of finding a particle at a particular point is proportional to the square of the wave function at the point.

* If $\psi(x)$ is the wave function of particle, then the probability of finding the particle within the range from x to $x+dx$ is $p(x)dx = \psi^*\psi\,dx = |\psi|^2 dx$.

where ψ^* is the complex conjugate of ψ.

* The total probability of finding the particle must be unity. $\int_{-\infty}^{\infty} p(x)\,dx = \int_{-\infty}^{\infty} \psi^*\psi\,dx = \int_{-\infty}^{\infty} |\psi|^2 dx = 1$

The electron probability (or) radial probability function (D) of a spherical shell is given as

$$D = \text{Volume of spherical shell} \times \psi^2$$

$$D = 4\pi r^2 dr \cdot \psi^2.$$

When $r=0$ (or) ∞, $D=0$, i.e. there is no probability of finding the 1s electron at the nucleus ($r=0$) & infinite distance ($r=\infty$) when $r = 0.529\,A^\circ$, $D = 95\%$. The electron is maximum probability of finding the electron at the Bohr's 1 orbit.

The Schrodinger Equation for Hydrogen Atom:

It is a 3 dimensional system & the Schrodinger equation for this system is

$$\hat{H}\psi = E\psi \quad \text{—— ①}$$

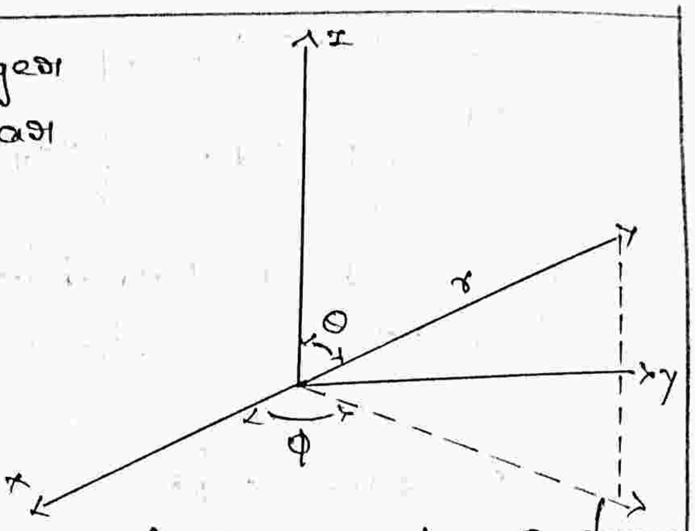
$$\hat{H} = \frac{-\hbar^2}{2m}\nabla^2 + V(x,y,z) \quad \text{—— ②}$$

$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ is Laplacian operator in the

Potential Energy of interaction between the electron & the nucleus is given by.

$$V(r) = \frac{-Ze^2}{4\pi\varepsilon_0 r}$$

Since the attractive potential has spherical symmetrical expanding only upon r, it is convenient to express the schrodinger equation in terms of polar co-ordinates (r, θ, ϕ), rather than cartesian co-ordinates.



$$x = r\sin\theta\cos\phi$$

$$y = r\sin\theta\sin\phi$$

$$z = r\cos\theta$$

The schrodinger equation for hydrogen atom in terms of polar co-ordinates become.

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(\frac{r^2\partial\psi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\cdot\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2} \quad \text{③}$$

$$+\frac{2\mu}{\hbar}(E-V(r))\phi=0.$$

μ - radial mass of electron & nucleus.

i.e. $\mu = \frac{m_e m_n}{m_e+m_n}$

$$\psi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi) \quad \text{④}$$

$R(r)$ - radial function, $\Theta(\theta)$ & $\Phi(\phi)$ - Angular function.

eqn ④ in ③ & multiplying by $\frac{r^2\sin^2\theta}{R\Theta\Phi}$

$$\frac{\sin^2\theta}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{\theta}\right)+\frac{2\mu}{\hbar^2}[E-V(r)]\,r^2\sin^2\theta$$

$$= \frac{-1}{\Phi}\frac{d^2\Phi}{d\phi^2} \quad \text{⑤}$$

$$\frac{d^2\Phi(\phi)}{d\phi^2} = -m^2\Phi(\phi) \quad \text{⑥}$$

& $\frac{\sin^2\theta}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\frac{2\mu}{\hbar^2}[E-V(r)]\cdot$

$r^2\sin^2\theta = m^2$ — ⑦

Dividing both sides by $\sin^2\theta$ & rearranging.

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2\mu}{\hbar^2}(E-V)r^2=-\frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\frac{d\Theta}{d\theta}\right)+\frac{m^2}{\sin^2\theta}$$ — ⑧

Then,

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\left(\lambda-\frac{m^2}{\sin^2\theta}\right)\Theta=0$$ — ⑨

& $$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2\mu}{\hbar^2}[E-V(r)]R-\frac{\lambda}{r^2}R=0$$ — ⑩

eqn ⑥, ⑨ & ⑩ called Φ equation, the Θ equation & the R-equation.

Nodal plane :-

Radial nodes (nodal surface) which is a hollow spherical region in which electrons cannot be.

Nodal plane (Angular Node) which is either a plane where electrons cannot be (or) conic surface.

Radial Node (Nodal surface) can be found Using the Principle (n) & Angular, Azimuthal (l) Quantum Number.

$n-l-1$

eg) 1s orbital.

$l=0$, $n=1$

so, $n-l-1 = 1-0-1 = 0$ radial node.

Angular nodes (nodal plane) can be found simply by determining l.

eg: => 2p orbital

l = 1 so, there is 1 angular Node.

l = 2 so, there is 2 angular Node.

=> 3p orbital

1 radial node = n-l-1 = 3-1-1 = 1

1 angular node l=1 so, 1

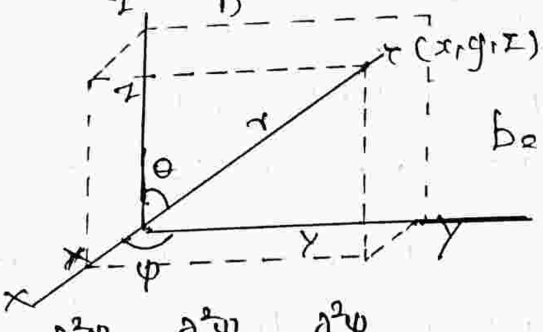
Radial & Angular functions:-

For most calculations, it is simpler to solve the Wave equation. if the cartesian coordinates x, y & z are converted into polar coordinates r, θ & φ

$$z = r\cos\theta \ , \ y = r\sin\theta\cdot\sin\phi \ , \ x = r\sin\theta\cdot\cos\phi$$

The schrodinger eqn is,

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



The relationship between cartesian & polar coordinates.

$$\nabla^2\psi = \frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}$$

Changing to polar coordinates, $\nabla^2\psi$ becomes.

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin^2\theta}\cdot\frac{\partial^2\psi}{\partial\phi^2} + \frac{1}{r^2\sin\theta}\cdot\frac{\partial}{\partial\theta}\cdot\left(\sin\frac{\partial\theta}{\partial\theta}\right)$$

The solution of this is of the form,

$$\psi = R(r), \Theta(\theta), \Phi(\phi)$$

R(r) is a function that depends on the distance from the nucleus, which in turn depends on the Quantum Number n & l.

Θ(θ) is a function of θ, which depends on the Quantum numbers l & m.

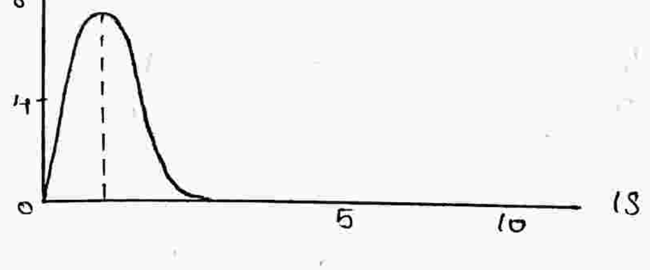
Φ(φ) is a function of φ, which depends only on the Quantum Number m. The eqn, $\psi = R(r)_{nl} A_{ml}$.

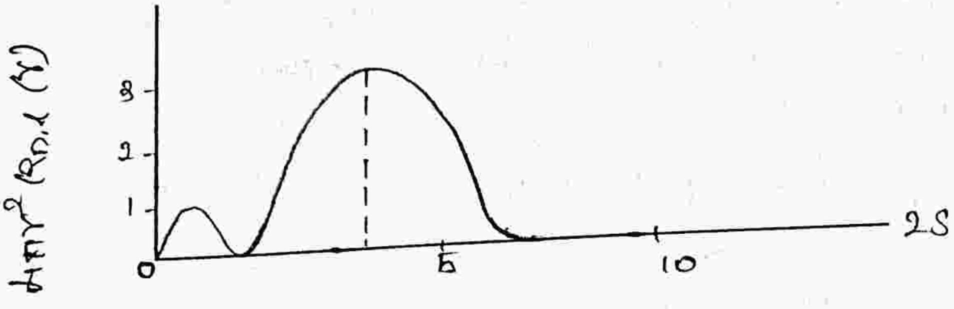
This splits the Wave function into two parts which can be solved separately.

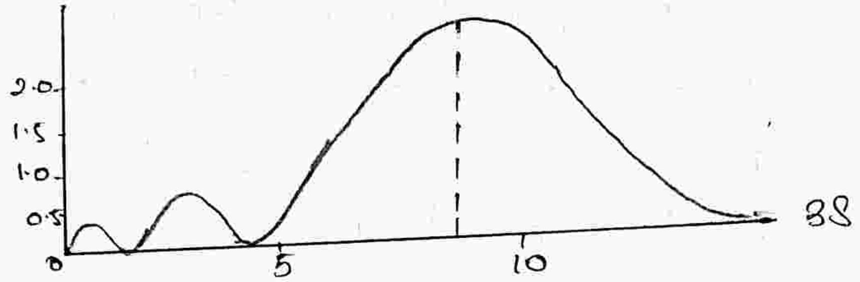
=> R(r) the radial function which depends on the Quantum Numbers 'n & l'

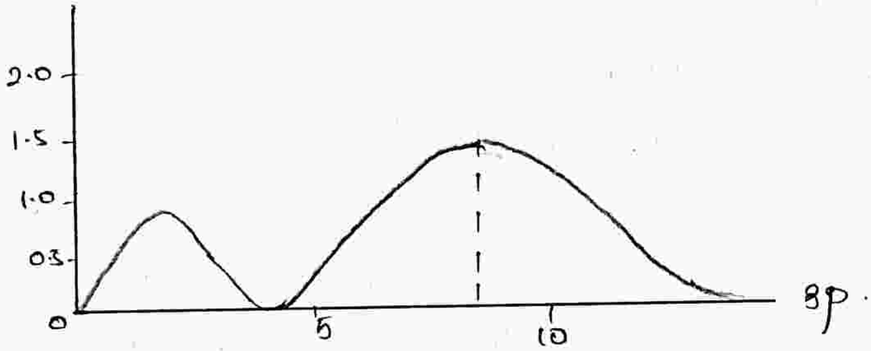
=> $A_{m,l}$ the total Angular Wave Function which depends on the Quantum Number 'm & l'

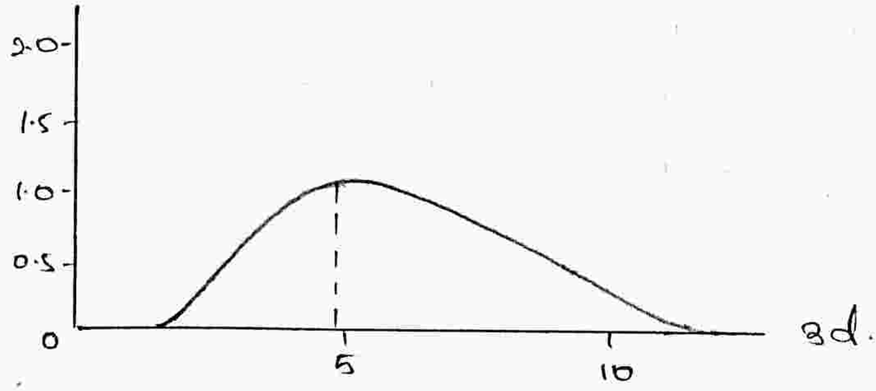
The radial function R has no physical Meaning. but R^2 gives the probability of finding the electron in a small Volume dv near the point at which R is measured. For a given Value of r the number of small Volume is $4\pi r^2$, so the probability of the electron being at a distance, from the nucleus is $4\pi r^2 R^2$. This is called the radical distribution function.




4πr² R_{n,l} (r)
3
2
1
0
5
10
2S


2.0
1.5
1.0
0.5
0
5
10
3S


2.0
1.5
1.0
0.5
0
5
10
3p.


2.0
1.5
1.0
0.5
0
5
10
3d.

The probability is zero at the nucleus ($r=0$) & the plots of 1s, 2s & 3s that the most π probable distance increases markedly at the principal Quantum Number increases. Further more, by comparing the plots for 2s, & 2p (or) 3s, 3p & 3d, it has been seen that the most probable radius decreases slightly as the subsidiary Quantum Number increases. except (1s) all others of 2s, 3s, 2p & 3d orbitals have shell like structure

The Angular function A depends only on the direction & is independent of the distance from the Nucleus (r). Thus, A^2 is the probability of finding an electron at a given direction, θ, ϕ at any direction from the nucleus to infinity.

Polar diagrams donot represent the total Wave function (ψ) but only the angular part of the Wave function.

The total Wave function,

$$\boxed{\psi = R(r)\cdot A}$$

Thus the probability of finding an electron simultaneously at a distance r & in a given direction, θ, ϕ is $\psi^2 r, \theta, \phi$.

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

Complete Wavefunctions for S orbitals & their shape:-

For an 'S' orbital $l=0, m=0$. So, complete wave function is

$$R_{n,0}(r)\, Y_0^0 = R_{n,0}(r) \frac{1}{\sqrt{2}} \times \frac{1}{\sqrt{2\pi}}$$

$$= R_{n,0}(r) \frac{1}{2\sqrt{\pi}} \quad \text{———} ①$$

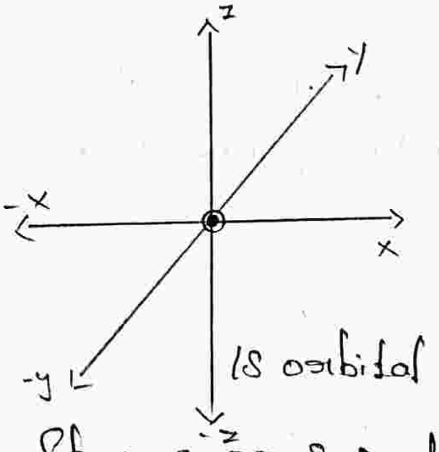
=> Independent of θ & φ

=> Spherical shape

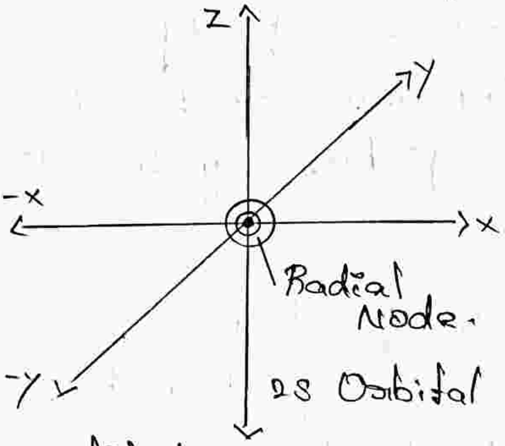
=> 1S has no radial node

=> 2S has one radial node

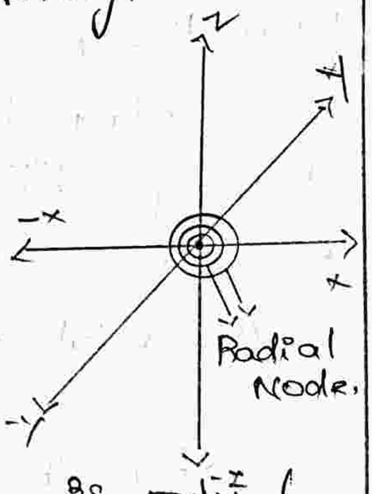
=> 3S has two radial nodes respectively.



1S orbital



2S Orbital

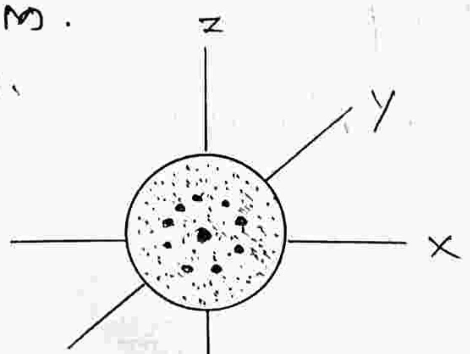


3S - orbital.

Shapes of S, p, d orbitals :-

The shape of orbitals depends on the Quantum Number l & m.

S - orbital :-

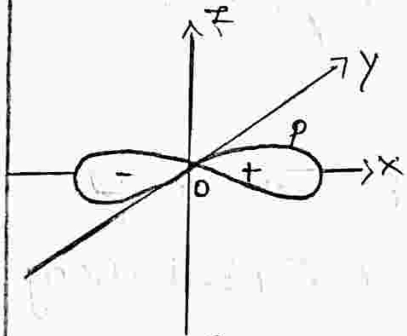


⇒ For s orbital $l=0, m=0$, there is only one orientation.

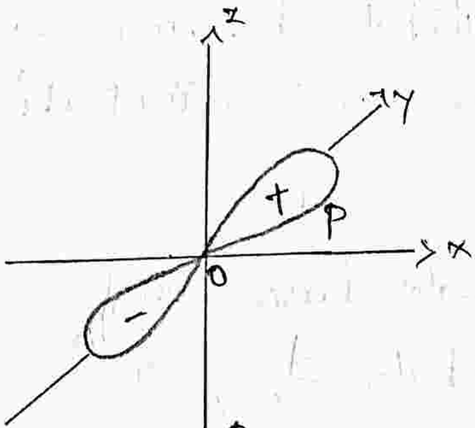
⇒ All s-orbitals are spherically symmetrical

⇒ The size of the orbital increases, as 'n' also increases.

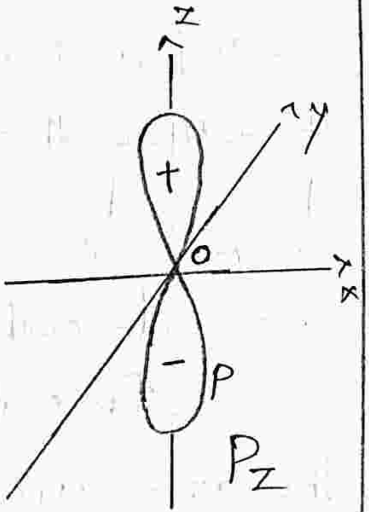
p- orbitals :-



P_x



P_y



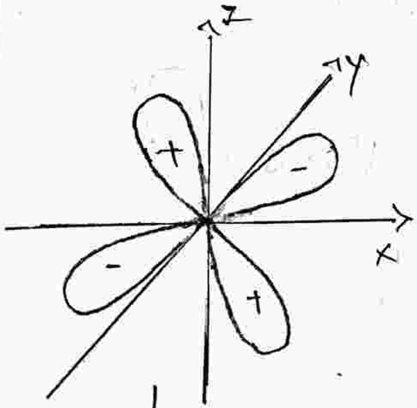
P_Z

⇒ For p-orbitals, $l=1$, m can have 3 values $-1, 0, +1$. Therefore there are 3 orientations P_x, P_y, P_z along the 3-axis.

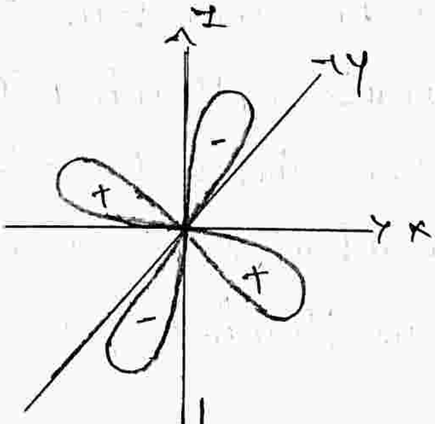
⇒ p-orbitals have dumb-bell shape.

⇒ Each orbital consists of two lobes separated by nodal plane.

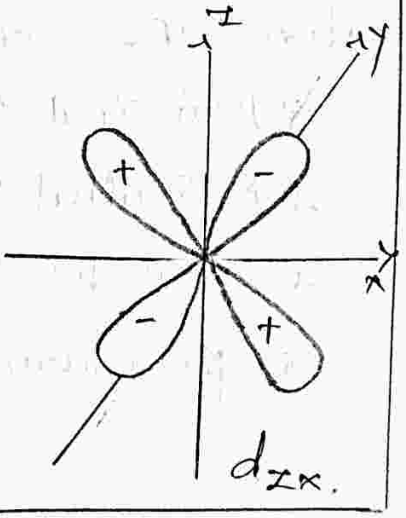
d- orbitals :-



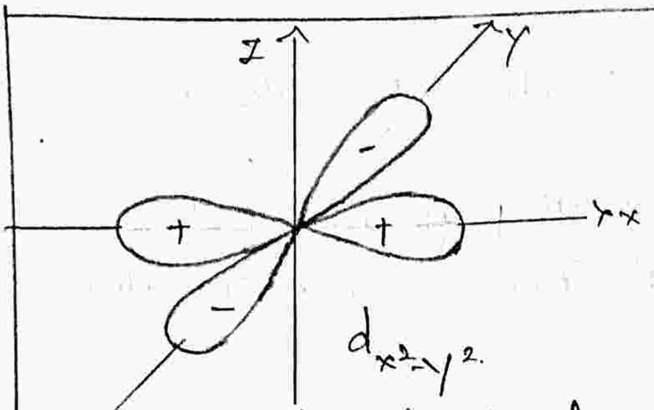
d_{xy}

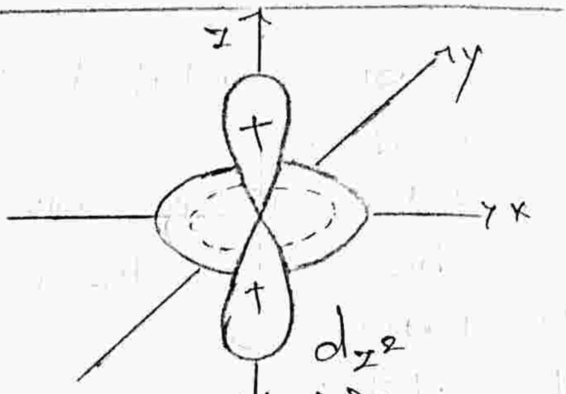


d_{yz}



d_{zx}





=> For d-orbitals $l = 2$, $m = -2, -1, 0, +1, +2$. Therefore there are 5 orientations d_{xy}, d_{yz}, d_{zx}, $d_{x^2-y^2}$, d_{z^2}

=> d-orbitals have double dumb-bell shape.

=> The orbitals $d_{x^2-y^2}$ & d_{z^2} are oriented along the axis (axial orbital)

=> The orbitals d_{xy}, d_{yz}, d_{zx} are oriented in between the cartesian axis (Non-axial orbital).

Quantum Numbers & its Significance:-

Solution of Schrodinger Wave equation involves some constants called Quantum Numbers. Quantum Numbers determine the Energy, shape, orientation & spin of the electron in an atom. There are 4 Quantum Numbers.

- * Principal Quantum Number (n)
- * Azimuthal (or) orbital Quantum Number (l)
- * Magnetic Quantum Number (m) &
- * Spin Quantum Number (s)

=> Principal Quantum Number (n) :-

Origin: Principal Quantum Number was proposed by Bohr to explain the origin of spectral lines.

Significance: Principal Quantum Number determines the main energy level of the electron. 'n' can take Values 1, 2, 3, 4 etc represented by K, L, M, N shells. The total Number of electrons in a given shell is calculated using the formula $2n^2$.

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

* It also determines the average distance of an electron from the nucleus.

=> Azimuthal Quantum Number (l)

Origin: This Quantum Number was introduced by Sommerfield to explain the fine structure of spectral lines.

Significance: Azimuthal Quantum Number described about the shape of the orbital. It is related to the angular Momentum of the electron. 'l' can have Values from 0 to n-1. The number of electrons in an orbital is given by the formula $2(2l+1)$.

l	orbital	shape	No. of electrons
0	s	spherical	2
1	p	dumb bell	6
2	d	double dumb bell	10
3	f	triple dumb bell	14

⇒ Magnetic Quantum Number (m).

Origin: Magnetic Quantum Number was introduced by Zeeman to explain the splitting of spectral lines in a Magnetic field (Zeeman effect).

Significance: Magnetic Quantum Numbers refers to different orientations of orbitals in space. For a given value of 'l' m can take values from $-l$ to $+l$ including zero. (i.e) $2l+1$ value.

l	m	orbital	orientations
0	0	s-orbital	1
1	-1, 0, +1	p-orbital	3 (p_x, p_y, p_z)
2	-2, -1, 0, +1, +2	d-orbital	5 (p_{xy}, p_{yz}, p_{zx}, $p_{x^2-y^2}$, d_{z^2}).

⇒ Spin Quantum Number (s).

Spin Quantum Number describes the direction of spin of the electron about its own axis. There are two possible directions. clockwise (or) Anti-clockwise. Hence 's' can take values $-\frac{1}{2}$ (or) $+\frac{1}{2}$.

Pauli's Exclusion Principle :-

It states that "No two electron in an atom can have all the four Quantum Numbers identical". If two electrons have same values of principal, Azimuthal & Magnetic Quantum Numbers then spin Quantum Number is different.

Illustration:

shell	n	l	m	S	Total no. of electrons.
K	1	0	0	$+\frac{1}{2}$	2
	1	0	0	$-\frac{1}{2}$	
	2	0	0	$+\frac{1}{2}$	8
	2	0	0	$-\frac{1}{2}$	
	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	$-\frac{1}{2}$	

Significance

* It is used to calculate the maximum no. of electron in a given shell.

eg:-

K shell	2
L shell	8
M shell	18
N shell	32

* The total no. of electrons present in any shell is equal to $2n^2$

* The principle shows that an orbital can occupy only two electron.

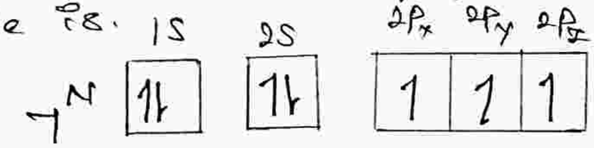
Hund's Rule:-

According to Hund's rule, "electron pairing in any orbit is not possible until the available orbitals contain one electron each".

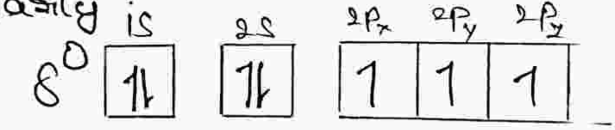
The filling up of electrons in a set of degenerative orbitals like P_x, P_y, P_z takes place such that there will be maximum number of unpaired electrons.

Illustration:-

Nitrogen with an electronic configuration $1s^2 2s^2 2p^3$ can have several electronic arrangement but the correct configuration according to Hund's rule is.



Similarly is



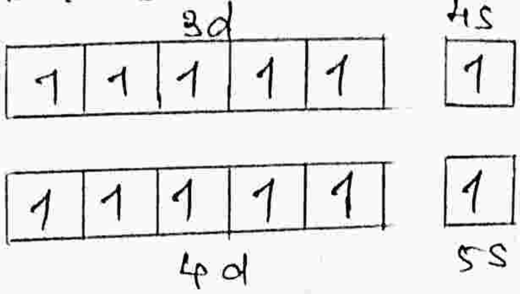
Significance:-

* Stability of half-filled orbital is a direct application of Hund's rule. In the half-filled state, electron have minimum repulsion & occupy low energy.

* The electronic configuration of Cr & Mo can be justified with the Hund's rule.

Cr (24) (Ar)

Mo (42) (Kr)



Aufbau Principle:-

According to Aufbau principle, "Electron enter the various orbitals in the order of increasing energy".

Electron occupy the orbitals of minimum energy first & then occupy the orbitals of higher energy.

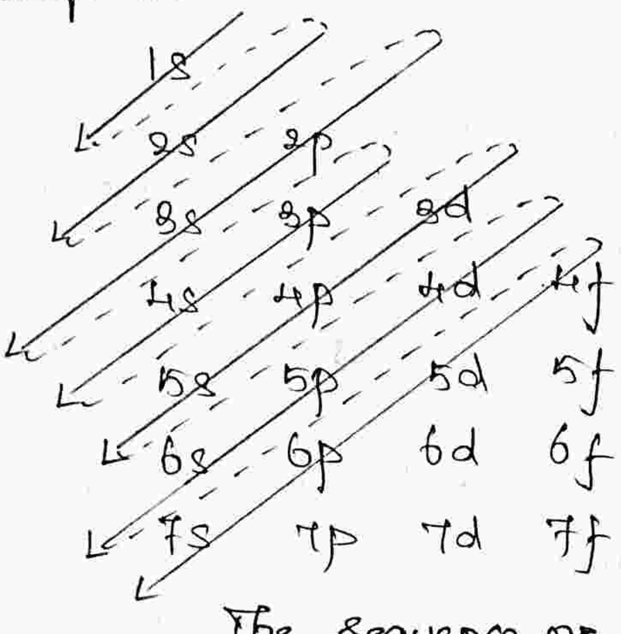
The order of filling up of orbitals is in accordance with the following rules.

=> Orbitals are occupied in the increasing order of their $(n+l)$ values.

=> When two (or) more orbitals have the same $(n+l)$ value, the one with the lower value of n, fills up first.

n	l	(n+l)	Orbitals.
1	0	1	1s
2	0	2	2s
	1	3	2p
3.	0	3	3s
	1	4	3p
	2	5	3d
4	0	4	4s

Electrons enter the orbitals in the following sequence.



The sequence of filling up of electrons in the orbitals -

$1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < 4d < 5p < 6s < 4f < 5d < 6p < 7s.$

Electronic configuration of some elements:

NAME	ATOMIC NO	ELECTRONIC CONFIGURATION:
Hydrogen	1	$1s^1$
Helium	2	$1s^2$
Lithium	3	$1s^2 2s^1$
Berelium	4	$1s^2 2s^2$
Boron	5	$1s^2 2s^2 2p^1$
Carbon	6	$1s^2 2s^2 2p^2$
Nitrogen	7	$1s^2 2s^2 2p^3$
oxygen	8	$1s^2 2s^2 2p_x^2 2p_y^1 2p_z^1$
Fluorine	9	$1s^2 2s^2 2p^5$
Neon	10	$1s^2 2s^2 2p^6$
Sodium	11	$(Ne)(3s^1)$
Magnesium	12	$(Ne) 3s^2$
Aluminium	13	$(Ne) 3s^2 3p^1$
Silicon	14	$(Ne) 3s^2 3p^2$
phosphorous	15	$(Ne) 3s^2 3p^3$
Sulphur	16	$(Ne) 3s^2 3p^4$
chlorine	17	$(Ne) 3s^2 3p^5$
Argon	18	$(Ne) 3s^2 3p^6$
Potassium	19	$(Ar) 4s^1$
calcium	20	$(Ar) 4s^2$
Scandium	21	$(Ar) 4s^2 3d^1$
Titanium	22	$(Ar) 4s^2 3d^2$
Vanadium.	23	$(Ar) 4s^2 3d^3$

NAME	ATOMIC No	ELECTRONIC CONFIGURATION.
chromium	24	$(Ar) 4s^2 3d^4$
Manganese	25	$(Ar) 4s^2 3d^5$
Iron	26	$(Ar) 4s^2 3d^6$
Cobalt	27	$(Ar) 4s^2 3d^7$
Nickel	28	$(Ar) 4s^2 3d^8$
Copper	29	$(Ar) 4s^2 3d^9$
Zinc	30	$(Ar) 4s^2 3d^{10}$.

Electronic Configuration of some ions:-

Sc [21]

Sc^{3+} [18] $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6$.

Ti [22]

Ti^{4+} [18] $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6$.

Relative Energies in Atomic Orbitals:-

The relative energies of various orbitals of single electrons depend on the value of principle Quantum Number 'n' & is independent of the value of azimuthal Quantum Number 'l'.

In Multi-electron atom, the energy of orbitals have the same values of 'n' different values of 'l'.

Thus both values of 'n' & 'l' determine the energy of an orbital.

Different orbitals having the same principle Quantum number 'n' may have different energies.

For a particular main energy level, the orbital having higher value of azimuthal Quantum Number 'l' has higher energy. In general, energies of orbitals belonging to the same main energy level follow the order $s < p < d < f$.

The orbital having lower $(n+l)$ value has lower energy. However for orbitals whose $(n+l)$ values of are equal, the orbital having lower value of 'n' has lower energy.

For example,

Energy Level for 4s orbital & 3d orbital.

$$\left.\begin{array}{l} 4s \Rightarrow n+l = 4+0 = 4 \\ 3d \Rightarrow n+l = 3+2 = 5 \end{array}\right\} \text{so, } 3d > 4s$$

3d higher energy than 4s orbital.

⇒ 4p & 3d orbital.

$$\left.\begin{array}{l} 4p \Rightarrow 4+1 = 5 \\ 3d \Rightarrow 3+2 = 5 \end{array}\right\} \text{Here we consider which one has higher principle Quantum Number}$$

so, here $4p > 3d$.

Anamalous Electronic Configuration :-

Some of the elements have electronic configuration that differ slightly from what our general procedure would lead us to predict. Because a few of these elements are important ones

It is useful to know their actual electronic configuration.

Equal Electron Configuration.

Element	Predicted Electron Configuration	Actual Electron configuration
Cu	[Ar] $3d^9 4s^2$	[Ar] $3d^{10} 4s^1$
Ag	[Kr] $4d^9 5s^2$	[Kr] $4d^{10} 5s^1$
Pd	[Kr] $4d^8 5s^2$	[Kr] $4d^{10}$
Au	[Xe] $4f^{14} 5d^9 6s^2$	[Xe] $4f^{14} 5d^{10} 6s^1$
Cr	[Ar] $3d^4 4s^2$	[Ar] $3d^5 4s^1$
Mo	[Kr] $4d^4 5s^2$	[Kr] $4d^5 5s^1$

2·PERIODIC TABLE

The periodic classification of the Elements:

It is An Important Contribution towards the Development Of chemistry. from time to time various Attempt have been made to arrange all known elements in Systematic manner.

The Various Attempt Include prout's Hypothesis, Dobereiner's traids, newland's Law of octaves, Lothar meyar's Atomic Volume curve and mendeleef's periodic Table.

Mendaleef's periodic Law and periodic Table:

According to mendaleef's periodic Law physical and chemical properties of elements are periodic function of their Atomic weight.

He Arranged the elements in Increasing order of their Atomic weight in form of table known as mendaleef's periodic table. Diving the Elements into group (vertial column) And periodic (horizontal rows)

The post mendaleef's development however, brought out a number of defects and Anomalies.

The work of mosely (1911) proved that properties of elements are well explained by Atomic Number rather than Atomic weights.

Modern periodic Law:

Physical And chemical properties of elements are periodic funtion of their atomic number.

This Eliminates the anomalies and defects of mendaleef's periodic table.

Long form of periodic Table:

* In long form of periodic table elements are grouped in the increasing order of atomic number (or) increasing orbital elements.

* This table is also called Bohr's periodic table as it reflecks the Bohr's classification of element into four types Based on electronic configuration.

* It is Derived from mendaleef's table by extending the long periodic and Introducing of the Transition elements in short period.

* The periodic table mly be divided into four main regions.

s block elements.
p block elements.

d block elements.

f block elements.

Based on filling of s, p, d and f levels.

5. PERIODS:

* Elements are arranged in several Horizontal rows called periods.

* Each period begins with Alkali metals and end with noble gas.

* The order in which Electron are filled in different energy levels correspons to number of electron in each period.

period	orbitals filled	Elements in the period.
1st	1s	2 H, He
2nd	2s, 2p	8 Li - Ne
3rd	3s, 3p	8 Na - Ar
4th	4s, 3d, 4p	18 K - Kr
5th	5s, 4d, 5p	18 Rb - Xe
6th	6s, 4f, 5d, 6p	32 Cs - Rn
7th	7s, 5f, 6d, 7p	incomplete period.

LONG FROM OF PERIODIC TABLE

S Block Elements.
(Representative elements)

D Blocks Elements.
(Transition elements)

← P Block Elements →
← (Representative elements) →

IA	IIA	IIIB	IVB	VB	VIB	VIIB	← VIIIB		→	IB	IIB	IIIA	IVA	VA	VIA	VIIA	VIIA
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 NE
11 Na	12 mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89 Ac	104 Ko	105 Ha	106 Unh.												

f block Elements (Inner transition Elements)

Lanthanides series →	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
Actinide series →	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

Group:

* The veritical columns in periodic table are called groups.

* According to IUPAC, Elements with one 's' electrons in valence shell are 1 (IA) Alkali metals and 2s are 2(IIA) alkaline earth metals. They are collectively called s block elements.

* In group 13(IIA), 14(IVA), 15(VA), 16(VIA), 17(VIIA) with valuence shell (p) They are collectively called p block elements.

* s and p block element are Representative elements.

* Elements La_{57} to Lu_{71} are called Lanthanides (4f block elements) and Ac_{89} to Lr_{103} are called Actinodes.

* They are collectively called Inner transition Elements.

merits of long from of periodic table:

* It is Based on Atomic number which is a fundamental property of elements.

* In this table classification elements is based on valence shell electronic configusation and hence it is more correct.

* noble gases with completely filled valence shell configuration is placed at extreme right in table.

It Represents a logic completion of each period.

* Noble gases act as bridge between highly Electronegative halogens and Electropositive Alkali metals.

* In this table of block elements are placed between S and P block elements.

* It explains similarities and gradation of properties of elements in terms of electronic configuration.

* In this table elements of two sub group are placed separately. Thus dissimilar elements do not come togethere.

* This table is easy to understand, remember and reprodeuse.

Demerits:

* The position of hydrogen is not clear.

* It fails to accomodate the Lanthanides and Actinides in main body of periodic table.

* The Inclusion lanthanum and Actinum along with Scandium and yettnium in Cgroup (III B) is not Justified.

* The periodic table does not reflect the exact Distribution of electrons among all the elements.

2.2 Classification of elements on the Basic of their electronic configuration:

Elements have been classified on basic of their electronic configuration into S, P, and d, f block elements.

1. S - Block Elements:

* It's the valence shell configuration can be written as ns^1 and ns^2 groups 1 (IA) and 2 (II A)

* Alkali and alkaline earth metals are called S block elements.

* They are metallic and highly electropositive

* It have low values of Ionisation energy. This is due to large size of Atom.

* They are good reducing agent.

* Electronic configuration of S block elements is given in following Table.

Group 1 (IA) Alkali metals	Group 2 (IIA) Alkali earth metals.
Li.... $2s^1$	Be.... $2s^2$
Na.... $3s^1$	mg.... $3s^2$
K.... $4s^1$	Ca.... $4s^2$
Rb.... $5s^1$	Sr.... $5s^2$
Cs.... $6s^1$	Ba... $6s^2$
Fr... $7s^1$	Ra... $7s^2$

2. P- Block element:

* The General electronic configuration of p-block elements Varies from (ns^2np^1 to ns^2np^6) ie) group (13 to 18) are called p Block elements.

* It have high value of Ionisation energy.
* They are highly Reactive.
* Electronic configuration of p block elements is given below.

13 (IIIA) ns^2np^3	14 (IVA) ns^2np^2	15 (VA) ns^2np^3	16 (VIA) ns^2np^4	17 (VIIA) ns^2np^5	18 (VIIIA) ns^2np^6
B	C	N	O	F	Ne
Al	Si	P	S	Cl	Ar
Ga	Ge	As	Se	Br	Kr
In	Sn	Sb	Te	I	Xe
Tl	Pb	Bi	Po	Ar	Rn.

D Block Elements:-

* The General electronic configuration of d block elements is $(n-1)d^{1 to 10} ns^2$
* Group (3 to 12) are collectively called d balck elements.
* The Electronic Configuration of first row transition Elements is Geiven below.

Elements.	Symbol	Atomic. No	Electronic configuration
Scandium	Sc	21	$[Ar] 4s^2 3d^1$
Titanium	Ti	22	$[Ar] 4s^2 3d^2$
Varadium	V	23	$[Ar] 4s^2 3d^3$
chromium	Cr	24	$[Ar] 4s^1 3d^4$
maganese	Mn	25	$[Ar] 4s^2 3d^5$
Iron	Fe	26	$[Ar] 4s^2 3d^6$
Cabalt	Co	27	$[Ar] 4s^2 3d^7$
Nickel	Ni	28	$[Ar] 4s^2 3d^8$

Copper	Cu	29	$[Ar]\ 4s^1\ 3d^9$
Zinc	Zn	30	$[Ar]\ 4s^2\ 3d^{10}$

There are four transition series characteristed by filling of 3d, 4d, 5d and 6d orbitals.

Groups	3	4	5	6	7	8	9	10	11	12
1st series	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
2nd series	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd
3rd series	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg

F-block Elements.

57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cr	99 Es	100 Im	101 Md	102 No	103 Lr

Lanthanides:

* Elements with atomic number (La_{57} to Lu_{71}) which are characterised by the filling of 4f level are called Lanthanides (Lu)

* The valuence shell electronic configuration of Lanthanides. may be represented as

$$4f^{0-14}, 5d^{0\ \text{or}\ 1}, 6s^2$$

Actinides:

* Elements from (Ac_{89} to Lr_{103}) are called Actinides

* The Valence shell electronic configuration of Actinides $5f^{0-14}, 6d^{1,2}, 7s^2$

Cause of periodicity:

* Elements with Similar properties occur at regular intervals in periodic table. Such elements fall to Same vertical coloumn.

ie) The same group.

* The Recurrence of Similar properties of elements at Regular intervals when they are arranged in Increasing order of Atomic Number is called periodicity.

Group 1	Group 17	Group 18
H $1s^2$	F--- $2s^2 2p^5$	He . $1s^2$
Li---- $2s^1$	Cl--- $3s^2 3p^5$	Ne---- $2s^2 2p^6$
Na---- $3s^1$	Br--- $4s^2 4p^5$	Ar---- $3s^2 3p^6$
K---- $4s^1$	I---- $5s^2 5p^5$	Kr---- $4s^2 4p^6$
Rb--- $5s^1$	Ar--- $6s^2 6p^5$	Xe--- $5s^2 5p^6$
Cs--- $6s^1$		Rn---- $6s^2 6p^6$.

* Elements showing periodicity of properties have the Same Valance Shell electronic configuration. Thus the cause of moreover, elements with Similar properties in periodic table. These Intervals are 2, 8, 8, 18, 18 and 32.

* These numbers corresponds to Numbers of elements in each period.

PERIODIC PROPERITES:

Properties such as atomic and Ionic radius, Ionisation energy, electron affinity, electron Nagativity etc...., which shows a variation across a period as well as in group are called periodic properties.

2.4 Atomic Radius:

* It is the distance between the centre of nucleus and electron cloud of outermost Shell.

It depends on Several factor such as
multiplicity of bond
covelent bonding. etc...,

It is studied under the following headings.

i) Covalent radius
ii) metallic radius
iii) vander walls radius.

i) Covalent Radius:

* covalent Radius of an Atom is equal to half internuclear distance Between two identical Atoms joined on Covalent Bond.

Example,

* The F-F Bond length 1.44Å ∴ The Covalent Radius of F=1.44/2 =0.72Å

For a Heteronuclear diatomic molecule, The single bond length is nearly the sum of covalent radius.

C=F bond length =1.49Å
Covalent Radius of C=0.77Å
∴ Covalent Radius Of F=1.49 -0.77
=0.72Å.

metallic Radius:

It is defined as one half of distance between the Atoms of metal in metallic closed a paket crystal lattice.

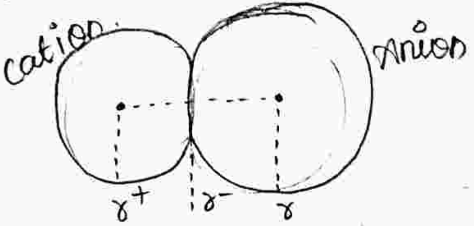
Vander walls radius:

Vander walls Radius is defined as one half of distance between the nuclear of two non bonded Isolated atoms.

Ionic Radius:

Ionic Radius is defined as distance between the nuclear of ion and point up to which the nucleaus has attraction over the electron cloud of ion. Interionic distance is sum of Ionic Radius of cation and anion

$d = r^+ + r^-$



periodic variation of Atomic and Ionic radius:

In period:

Atomic and Ionic Radius decrease from left to right across a period of normal elements.

Elements of 2^{nd} period	Li	Be	B	C	N	O	F
Covalent radii	1.23	0.90	0.82	0.77	0.75	0.73	0.72
Ionic radii	0.60	0.31	0.20	0.15	0.11	0.09	0.07
$A(M^+)$	(+1)	(+2)	(+3)	(+4)	(+5)	(+6)	(+7)

* In period, Electrons are added to same quantum levels while nuclear charge Increases by one.

* This Increase in nuclear charge is responsible for the Attraction of electron towards the nucleus.

∴ Covalent and Ionic radi decrease when we move from left to right in period.

* The Alkali metals have largest size and halogens have Smallest size.

* In case of d block element the Additional electron goes to penultimate shell. (n-1)

∴ decrease in size is only to small extent along a period.

In Group:

* On moving down the group both Atomic and Ionic radius Increase in Atomic Number.

Elements of Group (IA)	Li	Na	K	Rb	Cs
Covalent radius Å	1.23	1.54	2.03	2.16	2.35
No. of Shells.	2	3	4	5	6

when we move down a Group electrons are added to new Quantum level the number of shell Increases.

The No. of Shell Increase (↑)

∴ Atomic size Also Increase (↑).

In case of block elements, the Second and Third low transition elements have nearly same atomic and Ionic radius.

Covalent Radius of Transition Elements (Å)

Sc 1.44	Ti 1.32	V 1.22	Cr 1.17	Mn 1.17	Fe 1.17	Co 1.16	Ni 1.15	Cu 1.17	Zn 1.25
Y 1.62	Zr 1.45	Nb 1.34	Mo 1.29	Tc –	Ru 1.24	Rh 1.25	Pd 1.28	Ag 1.34	Cd 1.41
La 1.69	Hf 1.44	Ta 1.34	W 1.30	Re 1.28	Os 1.26	Ir 1.26	Pt 1.29	Au 1.34	Hg 1.44

Due to Lanthanide Contraction, the post Lanthanide elements have smaller size.

Ionisation Energy (Ionisation potential).

* Ionisation Energy is the energy recruired to Remove the most lossely bound electron from an Isolated gases us Atom.

M^{+} Energy $\rightarrow M^{+} + e^{-}$

* The first Ionisation energy is energy required to remove the first electron and convert (M to M^{+}) The second Ionisation energy is energy required to Remove the second electron and convert (M^{+} to M^{2+})

Hence,

$$\underset{\text{Increasing order}}{\underrightarrow{I_1 < I_2 < I_3}}$$

Veriation of Ionisation energy in period:

* In General Ionisation energy Increases when we move along a period from, left to right.

This is due to,

* Successive Increasing in Nuclear charge.
* Decrease in atomic size.

* In any period alkali metals have low Ionisation energies while halogens have high Ionisation energy.

Elements	Li	Be	B	C	N	O	F	Ne
Atomic no	3	4	5	6	7	8	9	10
I.E.K.J	520	900	800	1083	1403	1314	1081	2085

* The higher Ionisation energy of Be is due to compeletely filled 2S orbital.
* Removal of electron from filled 2S orbital is difficult and hence Ionisation energy of Be is Higher than Boron.
* The Ionisation Energy Become maximum for noble gase which has stable electronic configuration ns^2np^6
* The high value of Ionisation energy of nitrogen is attributed to half filled configuration.
* There is slight Increase in Ionisation energies of transiation elements when we move from group 3 to group 12.
* It is due to shielding of inner $(n-1)d$ electron.

Variation Of Ionisation Energy in a Group:

* Ionisation Energy decreases (↓) when we move from top to bottom in Group.

* The atomic size Increase, and attraction between the nucleus and outer electron decrease therefore Ionisation energy decrease.

ie, Ionisation Energies decreases (↓) in group.

Group 1 elements	Ionisation energies.
Li	520
Na	496
K	419
Rb	403
Cs	376

Group 2 elements	Ionisation energies.
Be	899
mg	737
ca	590
Sr	549
Ba	503

* In case D block elements Ionisation energies of 3rd transition series elements are higher than 1st and 2nd transition series elements.

* This is due to poor shielding of 4f orbital

Factors affecting Ionisation energy

i) atomic size:

* The Large size of atomic size the smaller in Ionisation energy (Reson: size of atom Increases the outer electron is Away from the Nucleus.

Atomic size —↑ (Increase)

Ionisation energy. ↓ (decrease).

ii) Nuclear Charge:

* The force of attraction between the Nucleus and outermost electron increase with Increase in Nuclear charge thus the greater the Nuclear charge the greater is energy needed to pull out an electron from atom.

* Hence Ionisation energy Increase with Increase in Nuclear charge.

iii) Number Of Electron in Inner Shells:

* The Large the number of electron in Inner Shells the smaller the Ionisation energy.

* The electrons in Inner Shell act as Screen (or) shield between the nuclear and electrons in outermost shell. This is known as screening effect or shielding effect.

* The Larger no of electrons in Inner Shell greater the screeing effect. Hence Ionisation Energy decrease (Low).

ELECTRON AFFINITY:-

* Electron affinity is also known as Electron gain enthalpy.

* It is defined as "Energy Released when an electron is added to valance shell of an Isolate gaseous atom to from a Negative Ion.

i) first electron affinity (EA1)

$$X(g) + e \rightarrow X + \text{Energy}.$$

* First electron affinity (EA1) is exothermic to the process as energy is Released.

ii) Second electron affinity (EA2)

* It is Energy required to add an electron to the uni negative gaseous ion.

$$X^{-}(g) + e^{-} + \text{Energy} \rightarrow X^{2-}$$

* Addition of electron to negative Ion leads to electrostatic repulusion, the process requires energy and hence EA2 is an endothermic process.

Factors affecting electron affinity:

i) Size of atom:

* In Small atom, the electrons are strongly held while in large atom, the electrons are less strongly held with nucleus there fore electron affinity decrease as size of atom

ie) size of atom - ↑ (Increase)
Electron affinity - ↓ (decrease).

i) Nuclear charge :

* Electron affinity depends on nuclear charge of atom. higher the nuclear charge. more strong is attraction between he nuclear and outer electron. Hence electron affinity increase with Increase in nuclear charge.

ii) Electronic configuration of atom:

* Atoms with stable electronic configuaration have no tendency to gain electron. There fore atoms with completely filled and half filled electron. configuration have nearly zero electron affinity.

* Atoms like (Be, Mg, N) etc... have zero E.A

* Similarly Noble gases have zero electron affinity.

variation of electron affinity in period:

* On moving from left to right in period the size of atom decrease and affective Nuclear increase. Hence electron affinity Increase when we move from left to right in period the alkaline metals have low values and halogens have high value of electron Affinities. ie) Electron afinity (↑)

variation of electron affinity in Group:-

* On moving down a group, size of atom Increase due to increase in no. of shells Hence electron affinity decrease when we go down a group.

ELECTRON NEGATIVITY:

* Electronegativity is tendency of atom to Attract the should pair of electron towards it self in covalent Bond.

Scales of electronegativity

pauling's scale:

* pauling's scale is based on partical ionic character of covalent Bond consider a covalent molecule AB If B is more electronegative the B gets a partial Negative charge and A gets partial positive charge

$$\boxed{A^{\delta+} - B^{\delta-}}$$

* Due to partial Ionic character the A-B Bond will be more stronger than a pure covalent Bond. The extra Bond energy A is

Δ = (Actual Bond energy) - (energy for 100% covalent bond)

* pauling suggested that 100% covalent bond energy is calculation as Geometrical mean of covalent Bond energies of A-A and B-B molecules.

$$\boxed{E\ 100\%\ \text{Covalent}\ A-B = \sqrt{E(A-A)-E(B-B)}}$$

$$\therefore \Delta = (\text{Actual Bond energy}) - \sqrt{E(A.A)-E(B-B)}$$

* Pauling Related Δ with electronegativity difference $(x_A - x_B)$ Between the bonded atoms as

$$x_A - x_B = 0.1017\sqrt{\Delta}$$

Δ is measured in $kJmol^{-1}$

ii) mulliken's Scale:

* Mulliken's Scale is based on Ionisation Energy and electron affinity of an atom.

* According mulliken Electronegativity of atom is average of Ionisation energy (I.E) and electron affinity value (E)

$$\text{Electronegativity} = \frac{(I+E)}{2}$$

Relation Between mulliken and pauling's Values:

* Mulliken measured I and E values in electron volt. The value was 2.8 times larger than pauling's values. If I and E are measured in $KJmol^{-1}$

$$I\ e.V/\text{mole} = 96.48\ KJmol^{-1}$$

$$\text{Electronegativity} = \frac{I+E}{2 \times 2.8 \times 96.48} = \frac{I+E}{540}$$

(iii) Allred and Rochow Scale:

* According to allred Rochow, Electronegativity is attractive force exerted by nuclear on valence electron

$$\boxed{F = -\frac{e^2 Z^*}{r^2}},$$

e = charge on an electron
r = covalent Radius.
Z^* = effective Nuclear charge.

* The F values may be converted to electronegativity by values using $\boxed{X = 0.749 + \frac{0.359 Z^*}{r^2}}$

* The electronegativity values calculated using the Above equation show close agreement with pauling's and mulliken's method.

Factors affecting Electronegativity:

i) Size of the atom:

* In a small atom, the Electrons are strongly hold with the nucleas and has greater tendency to attract electron Therefore small atoms have high value of electronegativity than large atoms.

ii) Effective nuclear charge:

* Electronegativity of an atom is proportional to effective nuclear charge

$$\chi \propto Z^*$$

∴ Electronegativity Increase with effective Nuclear charge.

iii) Ionisation energy and electron affinity:

* Electronegativity depends on values of Ionisation energy and electron affinity atoms with high Ionisation energy and electron affinity also have high values of electronegativity.

iv) Tybes of Hybritisation:

* Electronegativity Increase as the s-character of hybrid orbital Increase.

Variation of Electronegativity In period:

* On moving from left to right in period the size of the atom decrease and Effective nuclear charge Increase.

*Hence, The electronegativity Increase when we move from left to right in period.

* In periodic table halogens have maximum value of electronegativity.

Elements	Li	Be	B	C	N	O	F
Electronegativity.	1.0	1.5	2.0	2.5	3.0	3.5	4.0

Variation of electronegativity in Group:

* On moving down a group sized atom Increase. Hence Electronegativity decreased when we move down a group.

Group IA	Li	Na	K	Rb	C
Electronegativity.	1.0	0.9	0.8	0.8	0.7

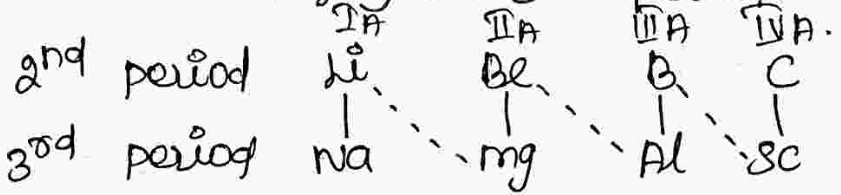
DIAGONAL RELATIONSHIP.

Definition:

* The Two elements showing similarities in properties are called diagonal relationship (or) diagonal neighbour.

* "Similarities in properties existing between the two elements of diagonal pair is known as diagonal Relationship"

* Diagonal Relationship is the Resemblance of properties of elements of 2nd period with diagonally opposite member lying in 3rd period.



3 diagonal pair (Li-mg) (Be-Al) (B-SC).

* The Two Elements of Diagonal pair is Bridge element. Both the Elements of each diagonal pair differ dignificanly in many properties from the other members of their own sub group But they show many pronouced Similarity with the elements situated diagonally opposite to them.

diagonal Relationship can be explained on Basic of 2 factors.

1. polarisation of ions
2. Electronegativity.

1. polarisation of ions.

* On moving from left to right in period at size decreases ∴ positive charge on cation Increase ∴ polarishing power (↑) Increase.

* On moving down group +ve charge on cation remain same but size (↑) Increase.

∴ polarishing power decreases.

* On moving diagonally in table. These two effect pactaly earicel each othe and a good similarity in proparties of 2 members of diagonal pair is observed.

2. Electronegativity:

* Electronegativity Increase from left to right in period and decrease along gp.

Be is more electronegative than Li

Be > Li
1.5 · 1.0

Mg shightly less electronegative than Be

Be > mg.
1.5 1.2

Li and mg being slightly less electronegative than Be have almost same value electronegativity.

∴ They have many Similar properties

∴ Hence they show diagonal Relationship with each other.

Z^* Effective nuclear charge:

* It is due to the Shilding effect of the Inner electron on the outer - electron that the valencen. electron less attractive pull from the nucleus.

* The decrease in attractive from reduce the nucleus charge this decreased nuclear charge is called affective Nuclear Charge (Z^*)

$Z^* = Z - \sigma$

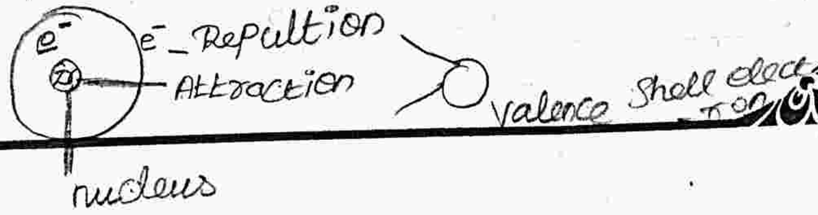
σ = Screening Constant / screening effect sheiding

Z = Atomic Number of element.

Shielding (or) Screening effect of Inner Shell electrons on valence Shell electron:

* In a multielectron atom the valence - Shell Electron are attracted by the nucleus and also at the Same time repelled by electron present between the nucleus and valence Shell electron.

(i e) Inner Shell electron.



* Thus the valence shell electron experience less Attraction (or) pull towards the nucleus:

Define:

* The decrease in attractive force exerted by the nucleus on valence shell electron, which is obviously. due to the presence of electrone clying between the nucleus and valence shell electrone is called shielding effect (or) screeing effect.

Factors affecting the magnitude of shielding effect.

① No. of Inner shell electron (or) Inner shell.

②. Types of orbital. occupied by the electrons.

① No. of Inner shell electron (or) Inner shell.

* In a Group the No. of Inner shell (or) Inner shell electrons Increase and hence the shielding effect also Increase.

Elements (IA)	Electronic configuration	No. of electrons in Inner shell	No. of Inner shells	order of shielding effect.
Li	2,1	2	1	↓ (↑)
Na	2,8,1	2+8=10	2	(↑)
K	2,8,8,1	2+8+8=18	3	(↑)
Rb	2,8,18,8,1	2+8+18+8=36	4	(↑)
Cs	2,8,18,18,8,1	2+18+18+8+8=54	5	Increasing

② Types of orbital occupied by the electrons:

* An electron in an s-orbital of given shell penetrates the nucleaor more strongly that in p-orbitals of same shell.

* penetration power decreasing ⟶

$ns > np > nd > nf$

value of n : same

* value of $l = 0, 1, 2, 3$ ⟶ Increasing so s-electron and more highly bound with the Nucleus that p-electron and p > d . due to the greater penetration power of s-electron it screens the nucleus more effectively than p-electron and soon

screening power decreasing ⟶

$ns > np > nd > nf$

matallic & Non metallic character of element

* metallic character - Electropositive.

* Non metallic character - electro negative

Matallic character:

Definition:

* It is defined as its tendency to loss one or more electron to form a cation.

$$M - ne^{\ominus} \longrightarrow M^{n+}$$

greater the tendency to lose ⟶ greater electropositive character ⟶ lesser the Ionization potential

∴ metallic character (↑)

∴ Ionisation potential / energy - (↓)

In group:

Ionisation energy decrease Hence, metallic character Increase. In group It is confirmed by the part that oxides of etc... of group become more and more base as we proceed from top to bottom in group.

∴ Na_2O_3, P_2O_3, As_2O_3, Sb_2O_3, Bi_2O_3

Acidic	Amphoteric (Both Acid Base)	Basic.

In period:

Ionisation energy Increase, Hence, metallic character decrease. In period it is confirmed by oxides.

Na_2O	MgO	Al_2O_3	SiO_2	P_2O_5	SO_3	Cl_2O_3
Strongly base	Base	Amphoteric	feebly acid	Acidic	more Acid	more Acidic

Non metallic character of elements.

Definition:

* It is defined as tendency to Accept one or more electron to form an anion.

$$M + ne^- \longrightarrow M^{n-}$$

Greater the tendency to gain e^- => greater non metallic character -> greater electron affinity.

In Group:

* Electron Affinity decrease (↓)

Hence, Non metallic character (↓)

In period:

* Electron Affinity Increase (↑)

Hence, Non metallic character (↑)

metals:

Elements lying at extreme left to periodic show minimum electronegative character they are called metals.

Non metals:

Elements lying at Extreme right of periodic table show maximum electronegative character they are Non metals.

Non metals.

IA	IIA	IIIA	IVA	VA	VIA	VIIA	zero
H							He
Li	Be	B	C	N	O	F	Ne
Na	Mg	Al	Si	P	S	Cl	Ar
K	Ca	Ga	Ge	As	Se	Br	Kr
Rb	Sr	In	Sn	Sb	Te	I	Xe
Cs	Ba	Tl	Pb	Bi	Po	At	Rn
Fr	Ra						

metalloids

how to calculate effective nuclear charge:

Example: 1

calculate the effective nuclear charge experienced by the 4S electron in potassium atom.

solution:

Electronic configuration of 'K' $= 1S^2 2S^2 2P^6, 3S^2, 3P^6, 4S^2$

Formula :-

$$\boxed{Z^* = Z - \sigma}$$

$= 19 - [0.85 \times$ No. of electrons in shell.$) + (1.00 \times$ total No. of electrons in inner shell)

$= 19 - [0.85 \times 8 + 1.00 \times 10]$

$= 19 - 16.8$

$Z^* = 2.20$

Variation of screeing effect in periodic table:

* The magnitud e of screeing effect also Increase in same direction on procedding from top to bottom of a Group and from left to right in period.

Element of Group (IA)	Li	Na	K	Rb	Cs
Value of Z :	3	11	19	37	55
Value of σ :	1.7	8.8	16.80	34.80	52.8

Elements of 2nd period	Li	B	B	C	N	O	F	Ne
Value of Z :	3	4	5	6	7	8	9	10
Value of σ :	1.7	2.05	2.4	2.75	3.1	3.45	2.8	4.15

Variation of Effective nuclear charge in periodic table:

In period:

From left to right across a period the atomic numbers [ie) Nuclear charge) Increase by one at each next element and next element has more valency electron with effective equal to 0.35 and ∴ The effective nuclear charge Increased by 1-0.35 = 0.65) from member to member.

The E.N.C of each atom is greader by 0.65 than then previous atom.

Example.

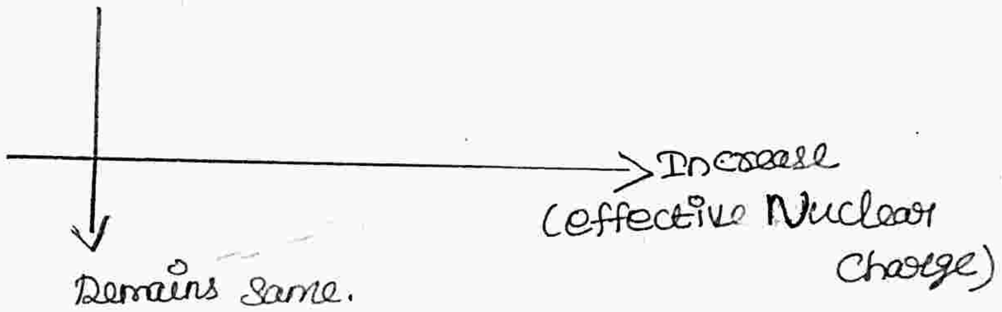
Elements of 2nd period.	Li	Be	B	C	N	O	F	Ne
Effective Nuclear charge :	1.3	1.95	2.6	3.25	3.9	4.55	5.2	5.85

In period effective nuclear charge Increase In group remain almost the same.

Example:

group 1A ⇒ Li = 1.80, Na = 2.20, K = 2.20, Rb = 2.20, Cs = 2.20, Fr = 2.20.

s block elements. p block elements.



Application:-

i) $1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 4s^2$ calculation of Effective Nuclear charge.

i) Z^*_{4s} = 19 − [0.85 × No. of electrons in (n−1) The shell + (100 × Total no. of electron in Inner Shell]

= 19 − [(0.85 × 8) + (100 × 10)]

= 2.20

ii) $1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 3d^1, 4s^0$

Z^*_{3d} = 19 − [1.00 × total no. of inner electron: ie) $1s^2 2s^2 2p^2$ 3p6 electrons]

= 19 − [1 × 18]

$= 19 - 18$

$= 1$

Effective Nuclear charge of 3d < E.N.C of 4S

Reason:

In K atom 3d electron is less highly bound to the nuclear than 4S electron so the additional electron perfer to enter 4S than 3d orbital.

① 4S orbital is filled before 3d orbitals.

② 4S electrons are removed before 3d electrons in the conversion of 3d transition elements into cations.

Electronic configuration of V $= 1S^2, 2S^2, 2p^6, 3S^2, 3p^6, 3d^3, 4S^2$

$V^{2+} = 1S^2, 2S^2 2p^6, 3S^2, 3p^6, 3d^3$

The Reason of 4S electron prefer to removed than 3d electrons can explained using. Z^*n

③ Successive Ionisation potential.

$(I_1 < I_2 < I_3)$ can explained E.N.C (effective Nuclear charge)

④ Atomic and Ionic radius: (S and P-block elements)

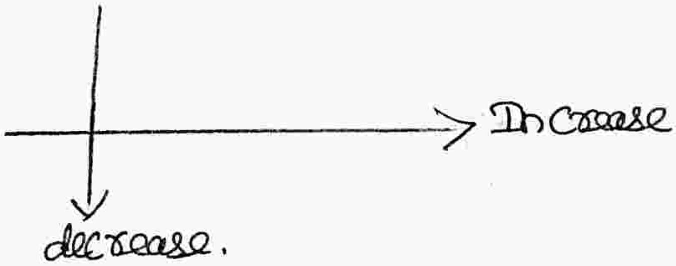
left to right decrease with Increase the atomic Number can be explained by effect Nuclear Charge. These are the Application of affect Nuclear charge.

Application of Electron Affinity:

① Tendency of elements to form Anion:

* In period Electron affinity Increase, the tendency of elements to accept the electrons and then to form the anion. Increase while the decrease of electron affinity values from top to bottom in group this tendency decrease.

S block elements p-block elements.



②. Oxidising power of elements:

* If an element in gaseous state $M(g)$ gain one electron and is converted in $(M^-(g))$. The element $m(g)$ is said to be acting are oxidising Agent.

$$M(g)+e^- \rightarrow M^-(g)$$

valency State(0) Lower valency State-1

*Thus the elements which have high electron Affinity values are strong oxidising agents.

*In Group electron Affinity Decrease.

*In period electron Affinity Increase.

* Halogens have maximum value of electron Affinity: Thus the oxidising power of halogens must be

$$F > Cl > Br > I$$

③ Non metallic character of elements:

It is defined as tendency to accept one (or) more elements to form an anion.

$$M + ne^- \longrightarrow m^{n-}$$

Non metallic character (↑)
Electron Affinity (↑)

④ Relative stability and Activity of elements:

i) The Ionisation potential Increase in periodbecause more energy is required to remove which mean Stablity of element. Increase.

ii) In Ionisation pontential decrease in Group because energy minimum is required to remove.
ie) stability of elements goes on decrease.

Hence, I.P – ↑ (Increase)
Stability also Increase.

Mulliken -Jaffe Electronegativities:

It indicates that an atom will be highly electronegativity if it releases much energy (because its energy curve is steep) as it acquires electron density, another atom will be less electronegative because its curve is less steep and, when combined with the more electronegative atom. It does not cost as much energy climbing its own energy curve. A molecule of ClF will exist as $Cl^{\delta+}F^{\delta}$, and it will be more stable than a hypothetical nonpolar ClF molecule.

Taking Eq. ① and subsituting $q=+1$, we know that the energy E, of the system will be that of the -1 cation, or the first ionization energy. Likewise for $q=-1$, the energy will be the negative[21] of the electron affinity.

$$IE_V = E_{+1} = \alpha(+1)+\beta(+1)^2 \longrightarrow ③$$

$$-EA_V = E_{-1} = \alpha(-1)+\beta(-1)^2 \longrightarrow ④$$

Subtracting Eq. 4 from Eq. 3 gives.

$$IE_v = EA_v = 2\alpha$$

*Which yields α as the mulliken electronegativity. The mulliken-jaffe definition of electronegativity for various hybridizations involves the computation of valence state ionization energies from valence state electron affinities by adjusting for the promotion energy from the ground state. The valence state ionization energy and electron affinity are not the experimentally observed values but those calculated for the atom in its valence state as it exists in a molecule.

*Divalent beryllium bonds through two equivalent, sp, or digonal, hybrids. The appropriate ionization energy therefore is not that of ground state beryllium $1s^2, 2s^2$, but an average of those energies necessary to remove electrons from the promoted, valence state.

$$1s^2 2s^1 2p^1 \rightarrow 1s^2 2s^1 \; (IE_p) \text{ and } 1s^2 2s^1 2p^1 \rightarrow 1s^2 2s^0 2p^1 \; (IE_s)$$

One of the strengths of the mulliken-jaffe approach is that it is capable of treading the electronegativity of partially charged atoms. we should not expect an atom that has lost electron density to have the same electronegativity as a similar atom that has not had such a loss, the former should be expected to hold on to its remaining electron density more tightly, conversely, as an atom acquires a partial negative charge. its attraction for more electron density more tightly. Conversely, as an atom readily by rewriting Eq. as its attraction for more electron density will decrease.

$$\chi = dE/d\delta = a + b\delta$$

First and Second Row Anomalies:-

In many ways the first ten elements differ considerably from the remaining.

Hydrogen belongs neither with the alkali metals nor with the halogen. athough it has some properties in common with both

It has +1 oxidation state in common with the alkali metals but the bare H^+ has no chemical existence and hydrogen tends to form covalent bonds that have properties more closely resembling there of carbon than those of the alkali metals.

with the halogens it shares the tendency to form a -1 oxidation state.

In contrast to the proton which was anamalous because of its small size the hydride ion is usually large. It is large than any of the halide tone except iodide.

Since the hydride ion is large and very polarizable it certainly does not extend the trend of I^- through F^- of decreasing size and increasing basicity and hardness.

*The elements of the second row also differ from their heavier longeners.

*Lithium is anomalous the alkali metals and resembles magnesium more than its congeners.

*G/P IA (2) Be ie more closely to aluminium than to the other alkaline earth.

fleurins is much more reactive than Cl, Br (or) I, Li is less reactive than its congeners.

*The most electronegative & smallest element of each family will he the one in the second rows.

$2\,LiOH \xrightarrow{red\ \Delta} Li_2O + H_2O$

$2\,NaOH \xrightarrow{\text{"}} Norkn$

$Li_2CO_3 \longrightarrow Li_2O + CO_2$

*The large ploarizable hydride ion which can bond more strongly by a covalent bond the lithium compound in the most stable.

Unit - 3

Sources of organic Compounds :

All organic Compounds Came from Plants (or) animals many of our most importants substance are still derived from these Sources directly (or) indirectly.

1, Plants and Animals :

Many organic Compounds are obtained directly from Plant and animals Sources by suitable method of isolation.

eg : 1. Carbohydrates cellulose , Sugar and Starches
2. Proteins Silk, wool , Casein
3. fat & oils Cottonsed Soybean oils , butter
4. alkaloids quinine , morphine , Strychnin
5. harmons , Vitamins , Perfumes , flavours and rasine.

2, Natural gas and petroleum :-

Natural gas and petroleum are now the major sources of organic compounds they are used as feels and also, through synthetic organic reaction for the production of hundreds of useful organic substance such as solvents, synthetic rubber, explosive and plastic.

3, Coal :-

Coal is major sources of organic compounds. It yield coke and coal-tar and pyrolysis (or) destructive distillation. more than 200 organic compounds have been directly isolated from coal-tar. these coal-tar products from the starting materials for the manufecture of thousands of useful aromatic compounds, including perfums, drugs, dyes, photographic developere.

4, Synthesis :-

Simple organic compounds derived from Petroleum (or) Coal have been Converted into thousands of useful materials by synthetic method. eg: organic compounds obtained from natural sources such as dyes, rubber, fibres, Plastic, drugs, Vitamins.

Nomenclature of organic compounds:

The earlier system of naming a Compound depends on the source from which it was obtained. Thus the names urea (from urine), methanol (meaning spirit of wood) and acetic acid (vinegar) were based on the sources of occurrence.

As the number of organic compounds increased enormously, it becomes difficult to assign trivial or common name to all new organic compounds. Hence the need for a systematic method of unambiguously naming organic compounds arises and it is called nomenclature.

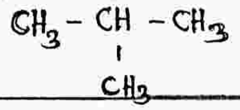
A chemical name has three parts in the IUPAC system. Prefix . Parent and Suffix. The Parent tells us how many carbon atoms are in the main chain and indicates the overall size of the molecule, the Suffix identifies the functional groups present in the molecule and the Prefix specifies the location of the functional groups and other subsituents on the main chain.

Prefix	Parent	Suffix
↓	↓	↓
Where are the substituents and functional groups?	How many carbons in the main chain?	What functional groups are present?

Alkanes or Paraffins or saturated hydrocarbons :-

These are compounds of carbon and hydrogen with general formula C_nH_{2n+2}. These compounds are

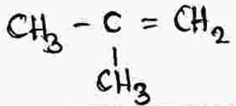
Characterised by linking Carbon atoms to each other through single bonds only.

	Stuctural formula	Common name	IUPAC name
1.	CH_4	Methane	Methane
2.	$H_3C - CH_3$	Ethane	Ethane
3.	$H_3C - CH_2 - CH_3$	Propane	Propane
4.	$H_3C - CH_2 - CH_2 - CH_3$	n - butane	Butane
5.	 $\underset{\displaystyle CH_3}{CH_3 - \underset{\vert}{CH} - CH_3}$	Iso butane	2-Methyl Propane .

Alkenes or olefins or unsaturated hydrocarbons :

The general molecular formula of an alkene is C_nH_{2n} . These compounds are characterised by the Presence of a Carbon - Carbon double bond $(\rangle C = C \langle)$

The IUPAC name is derived from alkanes by replacing the Suffix "ane" by "ene"

	Structural formula	Common name	IUPAC name
1.	$CH_2=CH_2$	Ethylene	Ethene
2.	$CH_3-CH=CH_2$	Propylene	Propene
3.	$CH_3-CH_2-CH=CH_2$	1 - Butylene	1 - Butene
4.	$CH_3-CH=CH-CH_3$	2 - Butylene	2 - Butene
5.	 $CH_3-\underset{\mid \atop CH_3}{C}=CH_2$	Isobutylene	2 - Methyl propene .

Alkynes:

The general molecular formula of an alkyne is C_nH_{2n-2}. These Compounds are characterised by the presence of a carbon - carbon triple bond $(-C\equiv C-)$. The names of the Compounds of this Series are derived from the name alkane Containing the Same number of Carbon atoms by replacing the Suffix "ane" by "yne".

Structural formula	Common name	IUPAC name
$H-C\equiv C-H$	Acetylene	Ethyne
$CH_3-C\equiv C-H$	Methylacetylene	Propyne
$CH_3-C\equiv C-CH_3$	Dimethylacetylene	2-Butyne
$CH_3-CH_2-C\equiv C-H$	Ethylacetylene	1-Butyne

Nomenclature of alkyl groups:

Straight - chain alkyl groups are formed by the removal of a terminal hydrogen atom from the straight - chain alkanes. These are named by replacing the suffix "ane" by "yl" Examples are.

CH_4 - Methane CH_3 - Methyl

CH_3-CH_3 - Ethane CH_3-CH_2 - or C_2H_3 Ethyl

It is equally possible to generate a number of branched alkyl groups by removing the internal hydrogen

Structural formula	Common name	IUPAC name
$H-C\equiv C-H$	Acetylene	Ethyne
$CH_3-C\equiv C-H$	Methylacetylene	Propyne
$CH_3-C\equiv C-CH_3$	Dimethylacetylene	2 - Butyne
$CH_3-CH_2-C\equiv C-H$	Ethylacetylene	1 - Butyne

Nomenclature of alkyl groups :

Straight - chain alkyl groups are formed by the removal of a terminal hydrogen atom from the straight - chain alkanes. These are named by replacing the suffix "ane" by "yl" Examples are.

CH_4 - Methane CH_3 - Methyl

CH_3-CH_3 - Ethane CH_3-CH_2 - or C_2H_3 Ethyl

It is equally possible to generate a number of branched alkyl groups by removing the internal hydrogen atoms from alkanes. For examples, there are two possible three - carbon alkyl groups and four possible four - carbon alkyl groups.

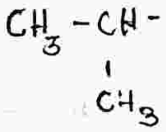
$CH_3-CH_2-CH_3$

Propane

$CH_3-CH_2-CH_2-$

n - Propyl

and



$CH_3-\underset{CH_3}{\underset{|}{CH}}-$

1 - Methylethyl (isopropyl)

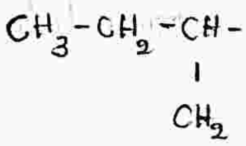
$CH_3-CH_2-CH_2-CH_3$

Butane

$CH_3-CH_2-CH_2-CH_2-$

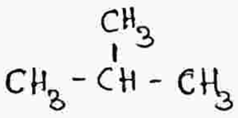
n - Butyl

and



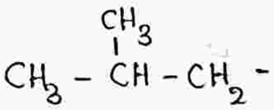
$CH_3-CH_2-\underset{CH_2}{\underset{|}{CH}}-$

1 - Methylpropyl (Sec-butyl)



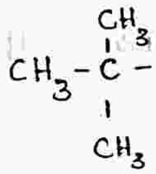
$CH_3-\overset{CH_3}{\overset{|}{CH}}-CH_3$

2 - Methyl Propane (Iso butane)



$CH_3-\overset{CH_3}{\overset{|}{CH}}-CH_2-$

2 - Methyl propyl (Iso butyl)



$CH_3-\underset{CH_3}{\underset{|}{\overset{CH_3}{\overset{|}{C}}}}-$

1, 1 - dimethyl ethyl (tert - butyl)

Branched - chain alkyl groups can be systematically named as per IUPAC nomenclature. For historical reasons

Some of the simpler branched - chain alkyl groups also have non - systematic or common names.

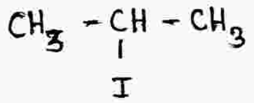
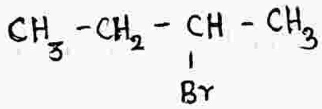
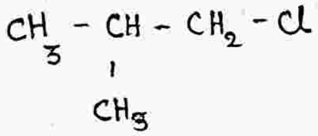
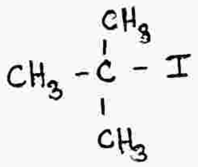
Alkyl groups containing double bonds

(i) $CH_2 = CH -$ Vinyl

(ii) $CH_2 = CH - CH_2 -$ Allyl

Alkyl halides

The general formula of alkyl halides is R-X where R stands for alkyl group and "X" stands for halogen (F, Cl, Br, I). They are named by introducing the prefix halo (chloro, bromo, iodo, fluoro) to the name of the parent alkane.

Formula	Common name	IUPAC name
$CH_3 - Cl$	Methyl chloride	Chloromethane
$CH_3 - CH_2 - Br$	Ethyl bromide	Bromoethane
$CH_3 - CH_2 - CH_2 - Br$	n - Propyl bromide	1- bromopropane
 $CH_3 - \underset{\substack{\mid \\ I}}{CH} - CH_3$	Iso- propyl iodide	2 - indopropane
$CH_3 - CH_2 - CH_2 - CH_2 - Cl$	n - butyl chloride	1 - chlorobutane
 $CH_3 - CH_2 - \underset{\substack{\mid \\ Br}}{CH} - CH_3$	Sec- butyl bromide	2 - bromobutane
 $CH_3 - \underset{\substack{\mid \\ CH_3}}{CH} - CH_2 - Cl$	Iso butyl chloride	1- chloro 2- methyl propane
 $CH_3 - \overset{\substack{CH_3 \\ \mid}}{\underset{\substack{\mid \\ CH_3}}{C}} - I$	ter - butyl iodide	2 - iodo - 2 - methyl propane
$CH_3 - CH - Cl$	Vinyl chloride	Chloroethene
$CH_2 - CH - CH_2 - Cl$	Allyl chloride	3 - chloro - 1 - Propane

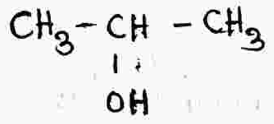
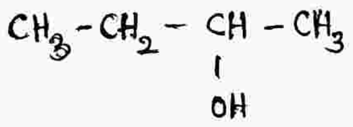
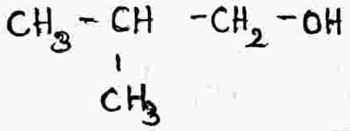
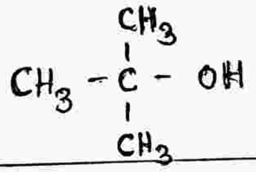
Alcohols :-

The term alcohols is applied to all organic Compounds obtained by replacing one or more hydrogen atoms of an open-chain hydrocarbon by hydroxyl groups. The alcohols are further classified into mono-, di-, tri-. hydric alcohols according to the number of hydroxyl groups which they may contain

In IUPAC nomenclature, the terminal "e" of the alkane is replaced by "ol".

Monohydric alcohols :-

Alcohols which Contain only one hydroxyl group per molecule are called monohydric alcohols.

Formula	Common name	IUPAC name
CH_3-OH	Methyl alcohol	Methanol
CH_3-CH_2-OH	Ethyl alcohol	ethanol
$CH_3-CH_2-CH_2-OH$	n- Propyl alcohol	1- Propanol
 $CH_3-\underset{\substack{\vert\\OH}}{CH}-CH_3$	Iso-Propyl alcohol	2- propanol
$CH_3-CH_2-CH_2-CH_2-OH$	n- butyl alcohol	2- butanol
 $CH_3-CH_2-\underset{\substack{\vert\\OH}}{CH}-CH_3$	Sec- butyl alcohol	2- butanol
 $CH_3-\underset{\substack{\vert\\CH_3}}{CH}-CH_2-OH$	Iso butyl alcohol	2-methyl-1-propanol
 $CH_3-\overset{\substack{CH_3\\\vert}}{\underset{\substack{\vert\\CH_3}}{C}}-OH$	tert-butyl alcohol	2-methyl-2-Propanol
$CH_2-CH-CH_2-OH$	Allyl alcohol	2- propane-1-01.

Dihydric alcohols :-

Alcohols which contain two -OH groups per molecule are called dihydric alcohols.

Structural formula	Common name	IUPAC name
CH_2-OH $\vert$ CH_2-OH	Ethylene glycol	1, 2- Ethanedio

Trihydric alcohols :-

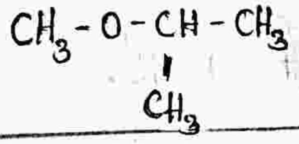
Alcohols which contain three -OH groups per molecule are called trihydric alcohols.

Structural formula	Common name	IUPAC name
CH_2-OH $\vert$ $CH-OH$ $\vert$ CH_2-OH	Gilycerol	1,2,3- Propane -triol

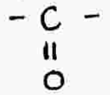
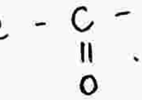
Ethers :-

An ethers is a Substance that has two organic groups bonded to the Same oxygen atom, $R-O-R'$. The organic group may be alkyl or aryl When the groups attached to the oxygen atom are the Same, they are termed as Simple ethers. When the groups attached to the oxygen atom are different, they are termed as mixed ethers.

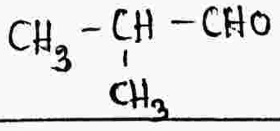
In IUPAC System, ethers are Considered to be alkoxy derivatives of hydrocarbons.

Structural formula	Common name	IUPAC name
Simple ethers		
CH_3-O-CH_3	Dimethyl ether	Methoxymethane
$CH_3-CH_2-O-CH_2-CH_3$	Dimethyl ether	Ethoxyethane
Mixed ethers		
$CH_3-O-CH_2-CH_3$	Ethyl methyl ether	Methoxyethane
$CH_3-O-CH_2-CH_2-CH_3$	Methyl n-Propyl ether	1-methoxypropane
 $CH_3-O-\underset{CH_3}{\underset{\vert}{CH}}-CH_3$	Iso Propyl methyl ether	2-methoxypropane

Aldehydes

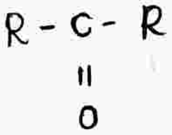
Aldehydes and ketones are two important Classes of Compounds Containing the Carbonyl group  $-\underset{\underset{O}{\|}}{C}-$ In aldehydes the  $-\underset{\underset{O}{\|}}{C}-$. group is linked to an alkyl group and a hydrogen or two hydrogens. Aldehydes are represented by the general formula R-CHO

IUPAC names of aldehydes are obtained by replacing the terminal "de" of alkane with "al"

Structural formula	Common name	IUPAC name
$H-CHO$	Formaldehyde	Methanal
CH_3-CHO	Acetaldehyde	Ethanal
CH_3-CH_2-CHO	propionaldehyde	Propanal
$CH_3-CH_2-CH_2-CHO$	Butyraldehyde	1- Butanal
 $CH_3-\underset{\underset{CH_3}{\mid}}{CH}-CHO$	Iso butyric aldehyde	2-Methyl propanal

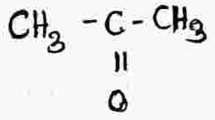
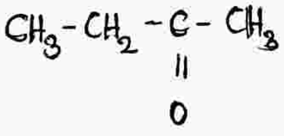
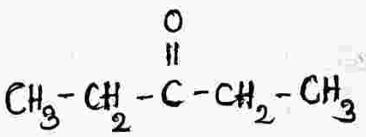
ketones :-

In ketones $-\underset{\underset{O}{\|}}{C}-$ group is united with 2 alkyl groups. These Compounds are represented by the general formula.



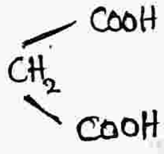
$$R-\underset{\underset{O}{\|}}{C}-R$$

Ketones are named by replacing the terminal "e" of the Corresponding alkane name with "one"

Structural formula	Common name	IUPAC name
 $CH_3-\underset{\underset{O}{\|}}{C}-CH_3$	Acetone Dimethyl ketone	Propanone
 $CH_3-CH_2-\underset{\underset{O}{\|}}{C}-CH_3$	Ethyl Methyl ketone	Butanone
 $CH_3-CH_2-\overset{\overset{O}{\|}}{C}-CH_2-CH_3$	Diethyl ketone	3- Pentanone

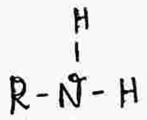
Carboxylic acids :

These are represented by the general formula R-COOH IUPAC name is derived by replacing the terminal "e" of the alkane name with "oic acid". These compounds are further classified into mono- and di-carboxylic acids.

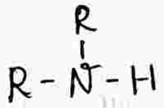
Structural formula	Common name	IUPAC name
Monocarboxylic acids		
$H-COOH$	Formic acid	Methanoic acid
CH_3-COOH	Acetic acid	Ethanoic acid
CH_3-CH_2-COOH	Propionic acid	Propanoic acid
$CH_3-CH_2-CH_2-COOH$	Butyric acid	Butanoic acid
Dicarboxylic acids		
$COOH$ $\vert$ $COOH$	oxalic acid	Ethanedioic acid
	Malonic acid	Propanedioic acid
CH_2-COOH $\vert$ CH_2-COOH	Succinic acid	Butanedioic acid

Amines :-

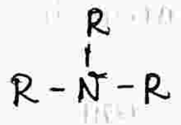
Amines are the derivatives of ammonia in which one or more H - atoms have been replaced by alkyl groups. They are designated as Primary. secondary and tertiary amines accourding as one, two or three hydrogen atoms in ammonia molecule have been replaced by alkyl groups



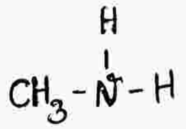
$R-\overset{H}{\overset{|}{N}}-H$



$R-\overset{R}{\overset{|}{N}}-H$

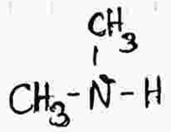


$R-\overset{R}{\overset{|}{N}}-R$



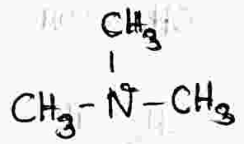
$CH_3-\overset{H}{\overset{|}{N}}-H$

Methylamine
(Primary amine)



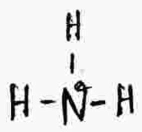
$CH_3-\overset{CH_3}{\overset{|}{N}}-H$

Dimethylamine
(Secondary amine)



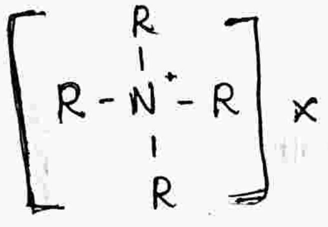
$CH_3-\overset{CH_3}{\overset{|}{N}}-CH_3$

Trimethyl amine
(tertiary amine)



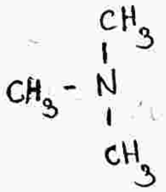
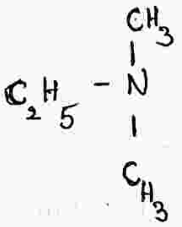
$H-\overset{H}{\overset{|}{N}}-H$

Ammonia



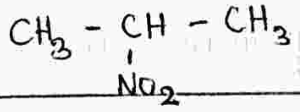
$\left[R-\overset{R}{\overset{|}{\underset{\underset{R}{|}}{N^+}}}-R\right]X$

quarternary Salt

Structural formula	Common name	IUPAC name
Tertiary Amines.		
 $CH_3-N(CH_3)-CH_3$	Trimethyl amine	(N, N - dimethylamino) methane
 $C_2H_5-N(CH_3)-CH_3$	Ethyl dimethyl amine	(N, N - dimethylamino) ethane

Nitro Compounds :-

These Compounds are represented by the general formula RNO_2 IUPAC names are obtained by adding the Prefix "nitro" to the alkane.

Structural formula	Common / IUPAC name
1. CH_3-NO_2	Nitromethane
2. $CH_3-CH_2-NO_2$	Nitroethane
3. $CH_3-CH_2-CH_2-NO_2$	1- Nitropropane
4.  $CH_3-CH(NO_2)-CH_3$	2- Nitropropane

When one alkyl group is attached to N- atom. It is called Primary amine, when two alkyl groups are attached to nitrogen atom then it is called Secondary amine. When three alkyl groups are attached to nitrogen atom it is called tertiary amine. When four alkyl groups are attached to nitrogen atom it is called quarternary salt.

	Structural formula	Common name	IUPAC name
	Primary Amines		
1.	$CH_3 - NH_2$	Methyl amine	aminomethane
2.	$CH_3 - CH_2 - NH_2$	Ethyl amine	aminoethane
3.	$CH_3 - CH_2 - CH_2 - NH_2$	n- Propyl amine	1-aminopropane
4.	$CH_3 - \underset{\underset{NH_3}{\mid}}{CH} - CH_3$	Iso Propyl amine	2- aminopropane
	Secondary Amines		
1.	$CH_3 - NH - CH_3$	Dimethyl amine	(N-methylamino) methane
2.	$CH_3 - CH_2 - NH - CH_2 - CH_3$	Diethyl amine	(N-ethylamino) ethane
3.	$CH_3 - NH - CH_2 - CH_3$	Ethyl methyl amine	(N- methylamino) ethane

Molecular Weight demination of organic acids and bases :-

Silver Salt Method :-

This methord is based on the fact that they form insoluable silver salts which upon heating decompose to leave a residue of metallic silver

Procedure :-

A small quantity of the unknown acid is dissolved in water and treated with a slight excess of ammonium hydroxide. The excess of ammonia is then boiled off. To this is added sufficient quantity of silver nitrate when a white precipitate of silver salt is obtained. The precipitate is seperated by filteration, washed successively with water, alcohol and ether and dried in the steam over. The dry silver salt is weighed into a crucible and ignited until all decomposition is complete ignition is repeated till the crucible with the residue of

Silver has attained constant weight. The molecular weight of the acid is then calculated from the weight of the silver salt taken and then weight of the residue of metallic silver obtained from it.

Calculation :-

Weight of the silver salt = xg

Weight of the residue of metallic silver } = ag

'a'g of metallic silver would leave from } = xg of silver salt

$\therefore$ 108g of metallic silver = $108 \times \frac{x}{a}$

$\frac{108 \times x}{a}$ is the equivalent weight of the silver salt of the acid.

Equivalent weight of acid } = Equivalent weight of silver salt - Equivalent weight of Ag + Equivalent weight of Hydrogen.

Equivalent weight of acid $\Big\} = \frac{x}{a} \times 108 - 108 + 1 = \frac{x}{a} \times 108 - 107.$

Molecular weight of acid $\Big\} =$ Equivalent weight × basicity

$$= \left(\frac{x}{a} \times 108 - 107\right) \times N.$$

Problem :-

1, 0.759 g of silver salt of a dibasic acid was ignited, when a residue of 0.463 g of metallic silver was left calculate molecular weight of the acid..

Weight of silver salt = 0.759 g.

Weight of silver left as residue $\Big\} = 0.463$g

The weight of silver salt would leave $\Big\} = 108$g of Ag

$$= \frac{0.759}{0.463} \times 108$$

$$= 177.05\text{g}.$$

This is equivalent weight of Silver Salt

The equivalent weight of the acid $= 177.05 - 108 + 1$

$= 70.05$

Molecular weight of the acid = Equivalent weight × basicity

$= 70.05 \times 2$

$= 140.1$

2, When heated cautiously is a crucible 0.3652g of Silver benzoate gave 0.1720g of Silver Salt. Find the molecular weight ?

The weight of silver benzoate = 0.3652g

Weight of Ag = 0.1720g

The weight of Silver Salt would leave } = 108g of Ag

$$= \frac{0.3652}{0.172} \times 108$$

This is equivalent weight of Silver Salt

$$= \frac{0.3652}{0.172} \times 108 = 229.2g$$

Equivalent weight of benzoic acid.

$$= 229.2 - 108 + 1 = 122.2$$

$$\left.\begin{array}{r}\text{Molecular weight of}\\ \text{benzoic acid}\end{array}\right\} = \text{Equivalent weight} \times \text{basicity}$$

$$= 122.2 \times 1$$

$$= 122.2$$

Platinichloride method for bases :-

Most organic bases (amines) combine with hydrochloroplatinic acid H_2PtCl_6, to form insoluable Salts known as Platinichloride. These double Salts may be represented by the general formula $B_2H_2PtCl_6$. Where 'B' Stands for one equivalent of the base. platinichlorides on ignition decomposes to leave a residue of Platinum.

$B_2H_2PtCl_6 \longrightarrow Pt$.

Knowing the weight of the Platinichloride taken and the platinum left behind the molecular weight of the base can be calculated.

Let 'x' g the weight of the Plantinicholoride taken and 'a' of the platinum residue ignition

Weight of Platinichloride = xg

$$\left.\text{Weight of the residue}\atop Pt\right\} = ag$$

'a' g of Pt is left by 'x' g Platinichloride

∴ 195g of Pt is left by $\frac{x}{a}$ g × 195 g Platinichloride

Equivalent weight of Platinichloride

$$= \frac{x}{a} \times 195$$

∴ The equivalent weight of the base, B

$$= \frac{\text{Equivalent weight of Platinichloride} - 410}{2}$$

$$= \frac{\frac{x}{a} \times 195 - 410}{2}$$

The acidity of the base is 'n' the molecular

weight of base = Equivalent weight × acidity

$$= \left(\frac{\frac{x}{a} \times 195 - 410}{2}\right) n$$

Problem :-

1. 0.6387 g of the Platinichloride of a monoacid base on ignition gave 0.209 g of Pt. Find the molecular weight of the base (Pt = 195)

0.209 g Pt is left by 0.6387 g of Platinichloride

∴ 195 g of Pt is left by $= \frac{0.6387 \times 195}{0.209}$

$\therefore$ Molecular weight of Platinichloride $= \frac{0.6387}{0.209} \times 195$

$= 596$

Equivalent weight of base $= \frac{\text{mol. of . Platinichloride} - 410}{2}$

$= \frac{596 - 410}{2} = 93$

Molecular weight of base = Equivalent weight x acidity

$= 93 \times 1 = 93$

2, 0.98 g of platinichloride of a diacid base left on ignition 0.3585 g of pt. Find the molecular weight of base

0.3585 g of Pt is left by 0.98 of Platinichloride

$\therefore$ 195g of Pt is left by $= \frac{0.98}{0.3585} \times 195$

Molecular weight of Platinichloride $= \frac{0.98}{0.3585} \times 195$

$= 533.$

$$\text{Equivalent weight of base} = \frac{\text{Molecular weight of Platinichloride} - 410}{2}$$

$$= \frac{533 - 410}{2}$$

$$= \frac{123}{2} = 61.53$$

$$\text{Molecular weight of base} = \text{Equivalent weight} \times \text{acidity}$$

$$= \frac{123}{2} \times 2$$

Molecular weight = 123.

Hybridization

Sp^3 HYBRIDIZATION OF CARBON

Let us Consider the electromic configuration of Carbon in its ground or atomic state

$$C\ (\text{Ground State}) = \frac{1s^2\ 2s^2\ 2p_x^1\ 2p_y^1\ 2p_z^0}{\text{Valence Shell}}$$

In terms of energy level diagram. this electron

Configuration may be represented as in Fig. 5.13. Since there are only two unpaired electrons (half - filled orbitals), it might be expected that only two single covlent bond will be formed.

On this basis, Carbon would combine with two hydrogen atoms ($H = 1S^1$) to form a molecule CH_2. The two C-H bonds would be formed by overlap of the 2p orbitals (P_x and P_y) with the 1s orbitals of each hydrogen atom. Since the angle separating the p orbitals is 90°, the C-H bonds would be at right angles to each other. But from chemical analysis we know that the simplest stable compound that Carbon forms with hydrogen is methane (CH_4) and this compound contains four identical C-H bonds.

Now let us assume that one of the 2s electrons in the ground state is moved or promoted to the empty P_z orbital Since $2P_z$ orbital is at a higher energy level than the 2s orbital this promotion process would require input of energy. This energy is supplied in the form of heat or light. This new state of Carbon is referred to as the **Excited State**. The electron configuration of the Carbon atom in its excited state is:

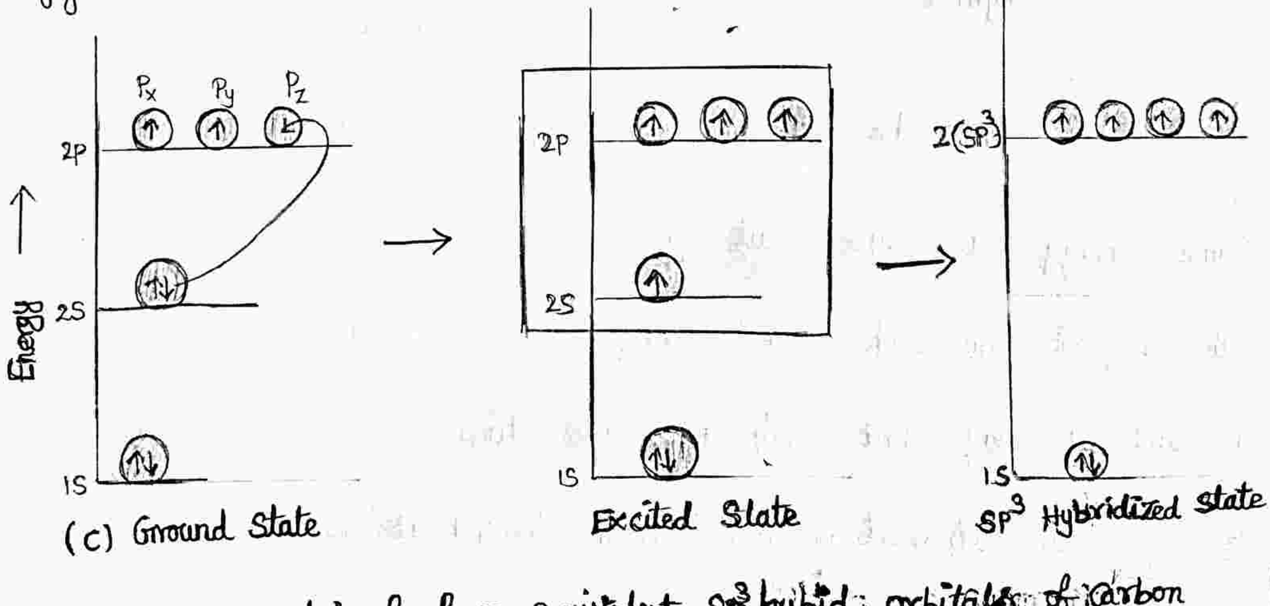
$$C\ (\text{Excited State}) = \frac{1s^2\ 2s^1\ 2p_x^1\ 2p_y^1\ 2p_z^1}{\text{Valence Shell}}$$

In terms of energy level diagram, this electron configuration may be represented as in Fig. 5.13. Since there are four unpaired electrons. (half - filled orbitals) in the Valence Shell of the Carbon atom in its excited state, it might be expected that four covalent bonds will be formed. . on this basis, Carbon would combine with four hydrogen atoms to form a molecule CH_4. The three C-H bonds would be formed by the overlap of three 2P orbitals (P_x, P_y and P_z) with the 1s orbital of each hydrogen atom. The fourth C-H bond will be formed by the overlap of the 2S orbitals of Carbon with the 1s orbital of a hydrogen atom. Since the angle separating the p orbitals in an atom is 90°, the three C-H bonds may be expected to be at right angles to each other. The fourth C-H bond involving the overlap of s orbitals will not have any directional characteristics because s orbitals are spherically symmetrical. This implies that two different types of C-H bonds are involved in the formation of methane molecule. This is not true. Experimentally, methane has been shown to contain four identical C-H bonds that are directed towards the corners of a regular tetrahedron.

To form four identical bonds, Carbon must contribute a set of four equivalent orbitals. This can be achieved if the 2s and the three 2p orbitals (P_x, P_y and P_z) in the excited state are mixed or hybridized to give four new equivalent orbitals. These new orbitals are known as sp^3 (pronounced ess-pee-three) hybrid oribitals or simply **sp^3 orbitals** because they are formed by the interaction of one s and three p orbitals. Mixing of a pure s orbital and three p orbitals is rather like mixing of a gallon of Pure red Paint and three gallons of white Paint to give four gallons of Pink paint. This Process of mixing of Pure orbitals to give a Set of new equivalent orbitals is termed Hybridization and the Carbon is Said to be in Hybridized State. The electron Configuration of the Carbon atom in its SP^3 hybridized State is :

$$C \text{ Hybridized State} = \frac{1S^2\ 2(SP^3)^1\ 2(SP^3)^1\ 2(SP^3)^1\ 2(SP^3)^1}{\text{Valence Shell}}$$

In terms of energy level diagram, the above electron Configuration may be represented as in Fig. 5.13.



(c) Ground State
Excited State
SP^3 Hybridized state

Fig 5.13. Formation of four equivalent sp^3 hybrid orbitals of carbon

The Process which lead to the formation of four equivalent sp^3 orbitals are summarized in Fig. 5.13.

Each sp^3 orbital contains one electron. Since each sp^3 orbital is obtained from one s and three p orbitals. it has 25% s-character and 75% p-character. As indicated, each sp^3 orbitals has a large lobe and a small lobe (Fig. 5.14)

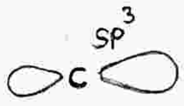


Fig. 5.14 Shape of an sp^3 hybrid orbital

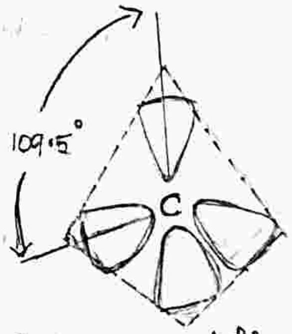


Fig 5.15 orientation of four sp^3 hybrid orbitals

The four new sp^3 orbitals obtained above are identical Same energy and shape but differ only in their orientation in space with respect to each other. The four sp^3 orbitals are arranged in such a way that their axes are directed towards the corners. of a regular tetrahedron with carbon located at the centre. The angle between any two orbitals is therefore 109.5°. The orientation of sp^3 orbitals is shown in Fig. 5.15. The smaller lobes are not indicated because they do not extend sufficiently far from nucleus to participate in bond formation.

The tetrahedral arrangement is favored because it allows the sp^3 orbitals to say as far away from each other as possible and thereby reducing the electron - electron repulsion. This is the keeping with the fact that each sp^3 orbital contains an electron and electron stay as far apart as possible because they have the same charge.

At this stage, the student should clearly understand that carbon does not necessarily undergo bond formation in its grounds state. The electron configuration may change prior to bond formation and the final arrangement that it acquries would depend upon the number of other atoms for groups to which it is attached.

Whenever Carbon is bonded to four other atoms or groups (as in methane), it uses SP^3 hybrid orbitals

Bonding in methane:

In methane Carbon forms single Covalent bonds with four hydrogen atoms. Since the Carbon atom is attached to four other atoms it uses SP^3 orbitals to form these bonds. Fig 5.16 Shows how the bonds in methane are formed.

Each C-H Covalent bond is the result of the overlap of an SP^3 orbitals from Carbon and 1s orbital from hydrogen.

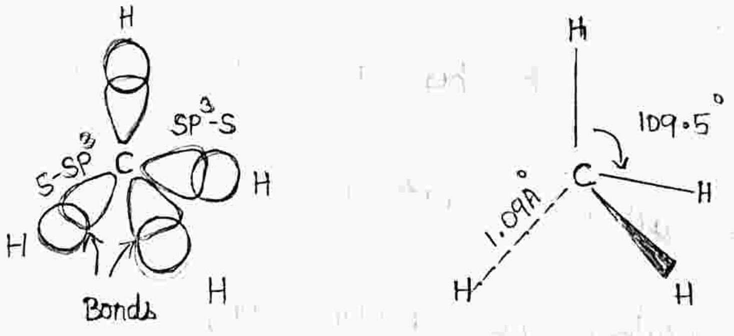


Fig. 5.16 Bonding in methane

Since the four SP^3 orbitals are oriented in such a way that their axes are directed towards the Corners of a regular tetrahedron with carbon located at the centre, the resulting C-H bonds are also directed towards the vertices of a tetrahedron with carbon at the centre. Thus, the bond angles in methane are the same as the angles between the axes of the sp^3 orbitals, that is 109.5°

The covalent bonds formed by the overlap of sp^3 orbitals and s orbitals are sigma (σ) bonds because the electron density in each bond is symmetrical about the line joining the centres of two bonded atoms. Thus all C-H bonds in methane are sigma bonds.

Electron diffraction and spectroscopic studies have shown that methane has a tetrahedral structure and all the C-H bonds are identical. They are the same length (1.09 Å). The energy required to break any of the four bonds is the same (102 kcal). The angle between any pair of bonds is 109.5°.

Bonding in Ethane :

In ethane there are six C - H Covalent bonds and one C - C Covalent bond. As in the Case of methane, each C - H bond is the result of the overlap of an sp^3 hybrid orbital from Carbon and Is orbital from hydrogen. The C - C bond arises from the overlap of sp^3 orbitals, one from each Carbon atom. Fig. 5.17 shows how the bonds in ethane are formed.

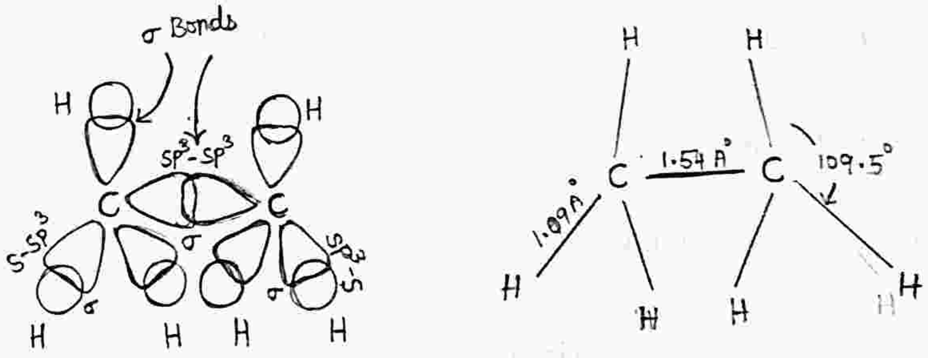


Fig. 5.17 Bonding in Ethane

All C - H bonds are the C - C bond are sigma(σ) bonds.

Electron diffraction and Spectroscopic studies have given the following measurements for the molecule of ethane : H - C - H and H - C - C bond angles are 109.5°, C - H bond length is 1.09 Å and C - C bond length is 1.54 Å

sp^2 HYBRIDIZATION OF CARBON

As in the Case of sp^3 hybridization, We start with the carbon atom in its ground State

$$C\ (\text{Ground State}) = 1s^2\ \underbrace{2s^2\,2p_x^1\,2p_y^1\,2p_z^0}_{\text{Valence Shell}}$$

The Promotion of one of the two 2s electrons to the empty p_z orbital gives the excited State.

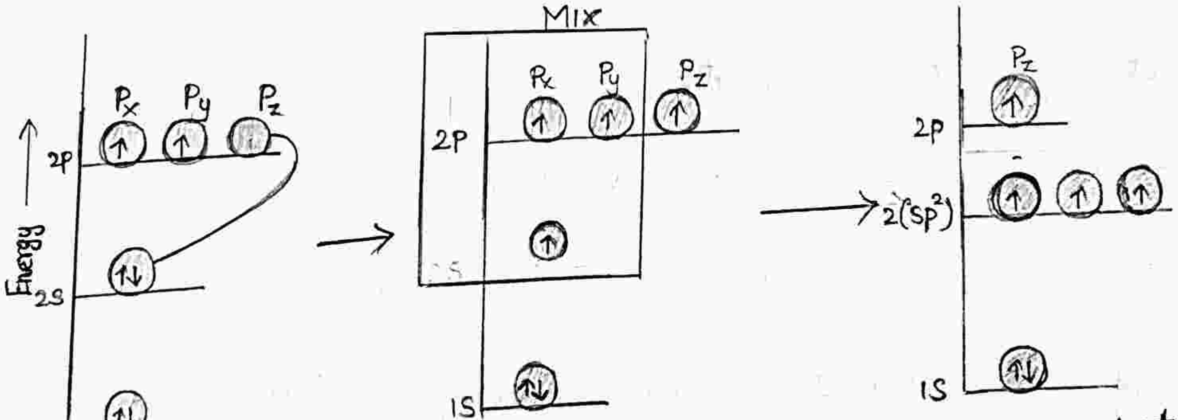
$$C\ (\text{Excited State}) = 1s^2\ \underbrace{2p^1\,2p_x^1\,2p_y^1\,2p_z^1}_{\text{Valence Shell}}$$

At this Point we follow a different Course than that used for sp^3 hybrization. in which Case one 2s and three 2p orbitals were mixed. Instead, the 2s electron and just two of three 2p orbitals are mixed or hybridization to give three new equivalent orbitals, These new orbitals are referred to as sp^2 (pronounced ess-pee - two) hybrid orbitals or Simply sp^2 orbitals. because they are formed by interaction of one s and two p orbitals. Third $2p_z$ orbital is left unhybridized. The electron configuration of the carbon atom in its sp^2 hybridized state is :

$$C \text{ Hybridized State} = 1s^2\ \underbrace{2(sp^2)^1\,2(sp^2)^1\,2(sp_z)^1}_{\text{Valence Shell}}$$

The Processes which lead to the formation of three equivalent sp^2 hybrid orbitals are summarized in Fig 5.18.

Each sp^2 orbital contains an unpaired electron. The shape of an sp^2 orbital is similar to that of an sp^3 orbital.



(C) Ground state Excited state sp^2- Hybridized State

Fig. 5.18. Formation of three equivalent sp^2 hybrid orbitals of carbon.

The Sp^2 orbitals obtained above are identical (Same energy and Shape) but differ only in their orientation in Space with respect to each other. The three sp^2 orbitals lie in the Same plane with their axes directed towards the Corners of an equilateral triangle. The angle between any pair of orbitals is thus 120°. The orientation of sp^2 orbitals with respect to each other is shown in Fig. 5.19 (a) The Smaller lobes are not indicated because they do not extend sufficiently far from nucleus to participate in bond formation. The trigonal arrangement is favored because it allows the sp^2 orbitals to stay as far apart from each other as possible and thereby reducing the electron-electron replusions.

The unhybridized P_z orbital is oriented along an axis Perpendicular to the plane of sp^2 orbitals, with each lobe above and below the plane of the sp^2 orbitals. Fig. 5.19 (c) indicates the position of the unhybridized P_z orbital in

The sp^2 orbitals obtained above are identical (Same energy and Shape) but differ only in their orientation in Space with respect to each other. The three sp^2 orbitals lie in the Same plane with their axes directed towards the Corners of an equilateral triangle. The angle between any pair of orbitals is thus 120°. The orientation of sp^2 orbitals with respect to each other is shown in Fig. 5.19 (a) The smaller lobes are not indicated because they do not extend sufficiently far from nucleus to participate in bond formation. The trigonal arrangement is favored because it allows the sp^2 orbitals to stay as far apart from each other as possible and thereby reducing the electron-electron replusions.

The unhybridized P_z orbital is oriented along an axis perpendicular to the plane of sp^2 orbitals, with each lobe above and below the plane of the sp^2 orbitals. Fig. 5.19 (c) indicates the position of the unhybridized P_z orbital in relation to the three sp^2 orbitals.

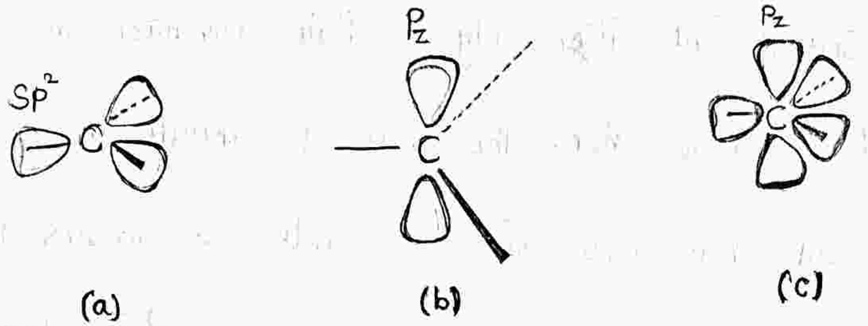


Fig 5.19 (a) orientation of three sp^2 orbitals. (b) The unhybridized P_z orbital. (C) orientation of the P_z orbital in relation to the sp^2 orbitals.

It should be remembered that whenever carbon is bonded to three other atoms or groups as in ethylene it always uses sp^2 hybrid orbitals and P_z orbital to form its bond.

Bonding in Ethylene :

Each carbon atom in ethylene ($H_2C=CH_2$) is attached to two hydrogen atoms by single covalent bonds and to another carbon atom by a double bond. Since each carbon is attached to three other atoms, it used sp^2 hybrid orbitals plus an unhybridized P_z orbital to form is bonds.

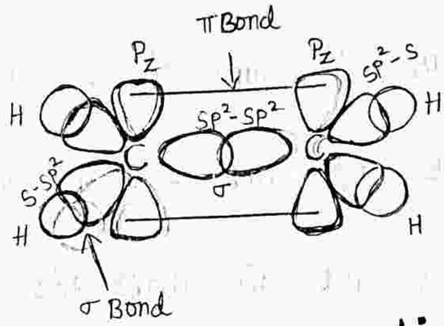


Fig. 5.20 Bonding in ethylene

In ethylene there are four C-H single covalent bonds and one C-C double bond. Each C-H bond is a sigma (σ) bond and results from the overlap of an sp^2 orbital from carbon and 1s orbital from hydrogen.

one of the two bonds in the double bond is also a σ bond and results from end-to end (linear) overlap of the sp^2 orbitals, one from each carbon atom.

The second bond in the double bond is a pi (π) bond and results from side-to-side (lateral) overlap of two unhybridized P_z orbitals, one from each carbon atom. It should be noted that P_z orbitals can overlap only when all six atoms lie in the same plane. that is the plane of the σ bonds. Like the p orbitals from which it is formed, a π bond consists of two equal parts. one part lies above the plane of the carbons and hydrogens and the other part lies below this plane. These two parts together make up one (π) bond.

Although the C-C double bond in the ethylene is represented by two equivalent lines remember that one lines represents a σ bond and the other the π bond (Fig.5.22)

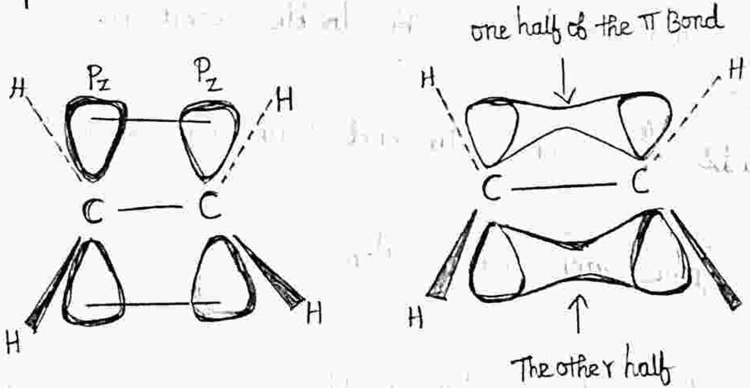


Fig: 5.21. Formation of the π bond in ethylene

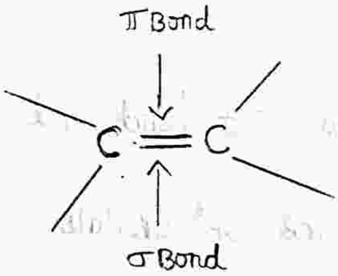


Fig: 5.22. The C-C double bond in ethylene is represented by two equivalent. one line represents a σ bond. The other line represents the π bond.

Electron diffraction and Spectroscopic Studies have also Shown that ethylene is a planar (flat) molecule. All bond angles (H-C-H and H-C-C) are 120°. The C-H bond length is 1.09 Å. The C-C bond length is ethylene is 1.34 Å as compared to the C-C bond length of 1.54 Å in ethane. This shortening is to be expected on the basis of additional orbital overlap associated with the two bonds.

Sp HYBRIDIZATION OF CARBON

As in the case of sp^2 hybridization, we again start with the carbon atom in its ground state

$$C \text{ Ground state} = 1s^2\ \underbrace{2s^2\ 2p_x^1\ 2p_y^1\ 2p_z^0}_{\text{Valence Shell}}$$

The promotion of one of the two 2s electrons to the empty p_z orbital gives the excited state.

$$C \text{ Excited state} = 1s^2\ \underbrace{2s^1\ 2p_x^1\ 2p_y^1\ 2p_z^1}_{\text{Valence Shell}}$$

At this point we fellow a different course than that used for SP^2 hybridization in which case one 2s and 2p orbitals were mixed, Instead, the 2s electron and just one of the three 2p orbitals are mixed or hybridized to give two new equivalent orbitals. These two new orbitals are referred to as sp (Pronounced ess-pee) hybridi orbitals or simply **sp orbitals** because they are formed by interaction of one s and one p orbital. The other two 2p orbitals (P_y and P_z) are left unhybridized. The electron configuration of the carbon atom in its sp hybridized state

$$C(\text{hybridized State}) = 1S^2 \underbrace{2(SP)^1\, 2(SP)^1\, 2P_y^1\, 2P_z^1}_{\text{Valence Shell}}$$

The Process which lead to the formation of two equivalent hybridized orbitals are Summarized in Fig. 5.23.

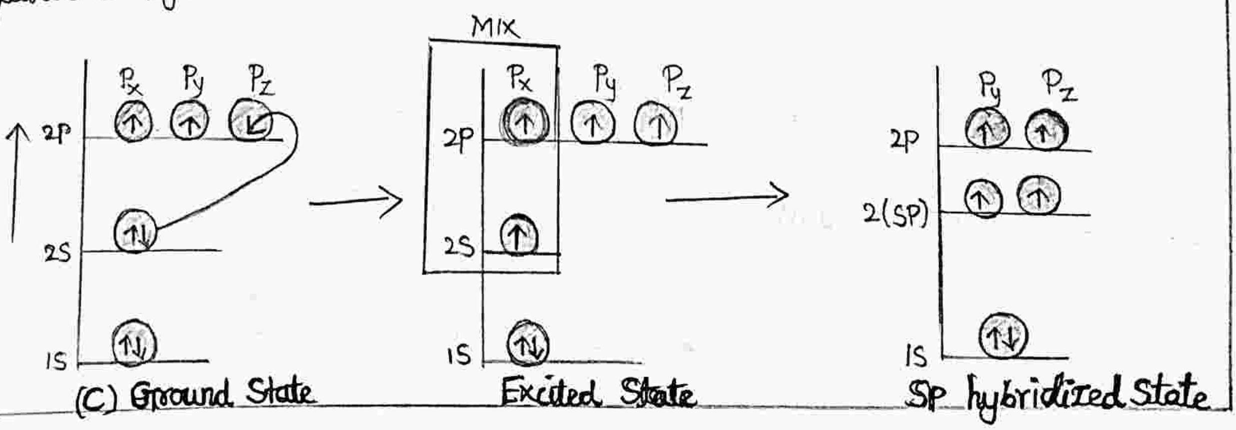
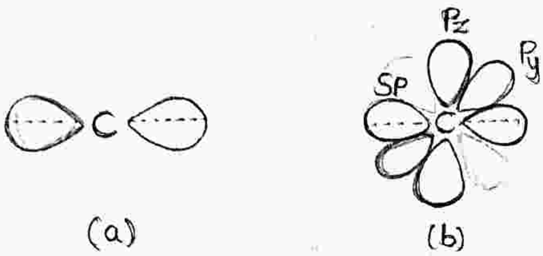


Fig. 5.23. formation of two equivalent sp hybrid orbitals of Carbon.



(a) (b)

Fig. 5.24. a) orientation of two sp orbitals (b) orientation of the unhybridized P_y and P_z orbitals in relation to the two sp orbitals

Each Sp orbitals Contains an unpaired electron. The Shape of an sp orbital is Similar to that of an sp^2 orbital. The sp orbitals obtained above are identical (Same energy and Shape but differ only in their orientation in Space with repect to each other. They lie in a Straight line. The angle between the two sp orbitals is thus 180° Fig. 5.24 a The linear arrangement is favored because it allows the sp orbitals. to Stay as far apart from each other as possible and thereby reducing the electron - electron replusions. The unhybridized P_y and P_z orbitals are at right angles to the line of the

Sp hybrid orbitals Fig. 5.24 (b) indicates the positions of the P_y and P_z orbitals in relation to the two sp orbitals.

It should be remembered that whenever Carbon is bonded to two other atoms or groups (as in acetylene) it always uses Sp hybrid Orbitals and two 2p (P_y and P_z) orbitals to from its bonds.

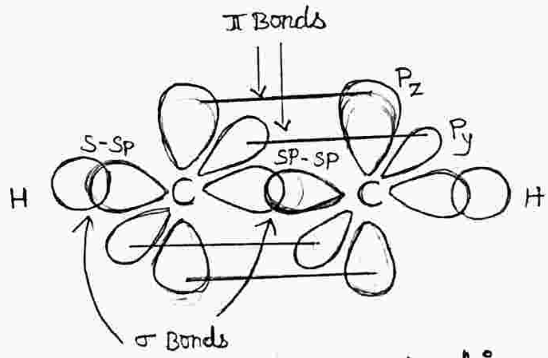


Fig. 5.25 Bonding in Acetylene

Bonding in Acetylene :

Each Carbon atom in acetylene ($H-C\equiv C-H$) is attached to one hydrogen atom by a Single Covalent bond and to another Carbon atom by a triple bond. Since each Carbon is attached to two other atoms it uses sp hybrid orbitals

Plus two unhybridized 2p orbitals (P_y and P_z) to from its bonds.

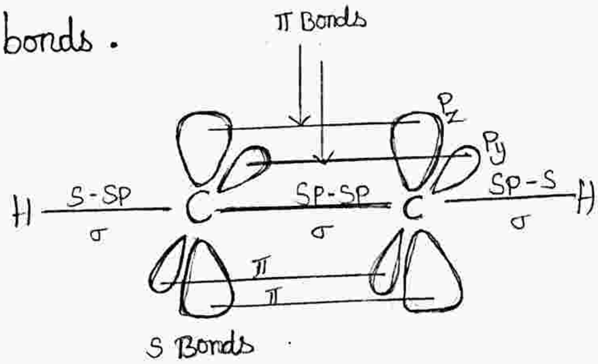


Fig. 5.26. Formation of the two π bonds in Acetylene

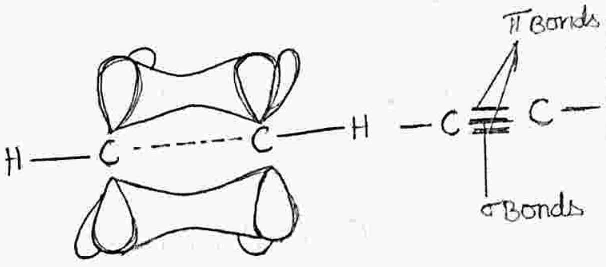


Fig. 5.27. The C-C triple bond in acetylene is representated by three equivalent lines. Two lines represent the π bonds. one line represents the bond.

In acetylene there are two C-H single covalent bonds and and one C-C triple bond. Each C-H bond is a sigma (σ) bond and results from the overlap of an sp orbital from carbon and 1s orbital from hydrogen.

one of the three bonds in the C-C triple bond is also a σ bond and results from end-to-end (linear) overlap of the two sp orbitals, one from each carbon.

The other two bonds in the triple bond are pi (π) bonds and result from Side-to-Side (lateral) overlap of the unhybridized p orbitals on each carbon.

Classification of organic Compounds

Oragnic Chemistry is the Study of carbon Compounds. Due to the Catenation Propery of Carbon, the Carbon atom Combines with other Carbon atoms to form large number of Compounds. The Study of these Compounds becomes easier by classifying Compounds into groups based on the Similaries of Structure and properties of the group members.

classification into open chain and cyclic

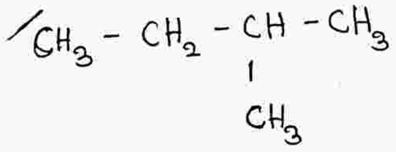
The organic Compounds are classified into two main types, namely.

1, open - Chain or acyclic Compounds or aliphatic

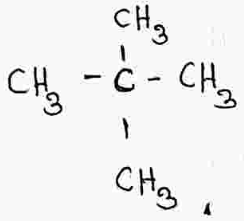
The open Chain or acychic Compounds are those in which carbon atoms are linked to each other either in linear or branched fashion Such that the molecule is having open chain Structure. These Compounds are also called aliphatic Compounds (Greek word : aleiphar meaning fat)

Examples :

$CH_3 - CH_2 - CH_3$ Propane



$CH_3 - CH_2 - \underset{\displaystyle CH_3}{\underset{|}{CH}} - CH_3$ 2- Methylbutane of isopentane



$CH_3 - \overset{\displaystyle CH_3}{\overset{|}{\underset{\displaystyle CH_3}{\underset{|}{C}}}} - CH_3$ neopentance

2, Closed chain or Cyclic Compounds :

organic Compounds with closed chain of atoms are called closed chain Compounds or ring

Compounds.

These Compounds are further classified into

* Homocyclic or Carbocyclic Compounds
* Heterocyclic Compounds.

a, Homocyclic Compounds :

In these Compounds the ring Structure is made up of only Carbon atoms.

These Compounds are further classified into

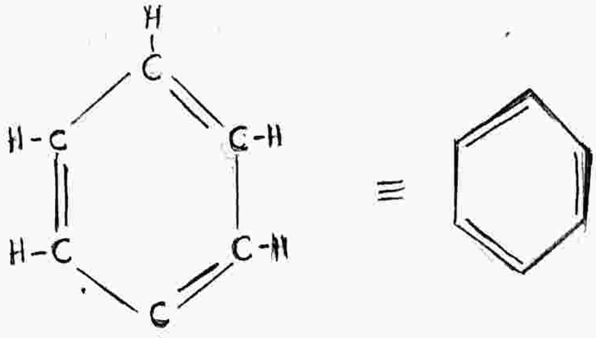
* Aromatic Compounds and
* Alicyclic Compounds.

i) Aromatic Compounds (Benzenoid)

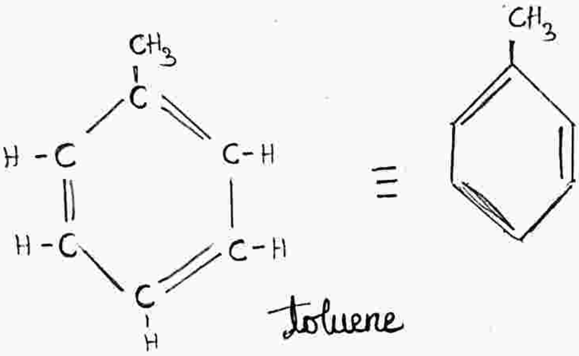
Compounds Containing one or more benzene rings in that Structure are classified as aromatic benzenoid Compounds. Most of these Compounds have Pleasant odour. (Greek : Aroma = Sweet Small)

Examples:

Monocyclic

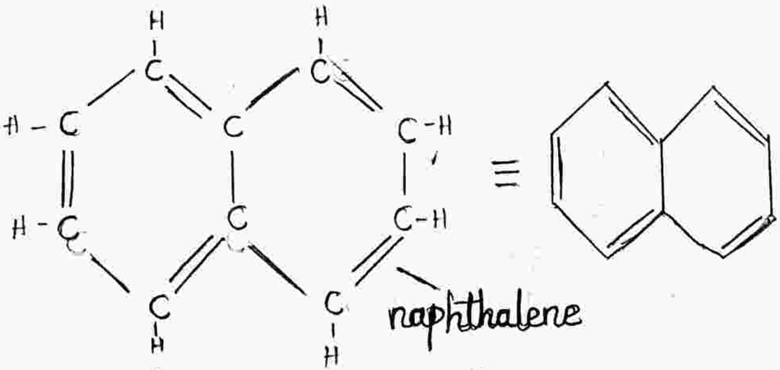


benzene

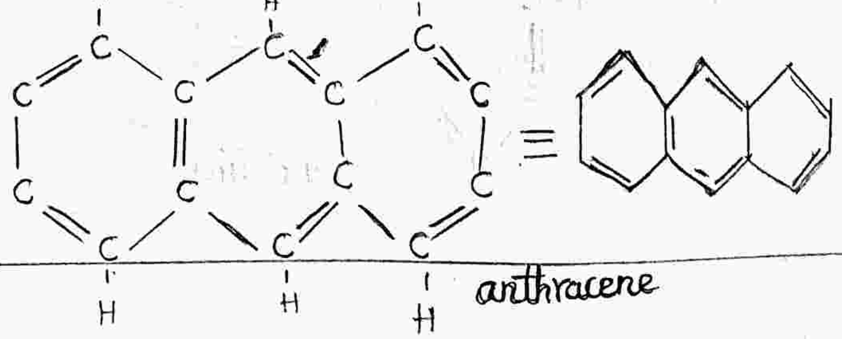


toluene

Polycyclic



naphthalene

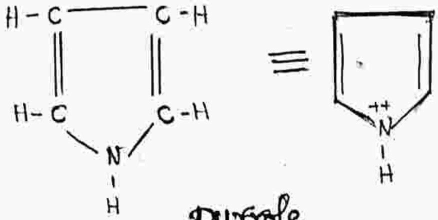


anthracene

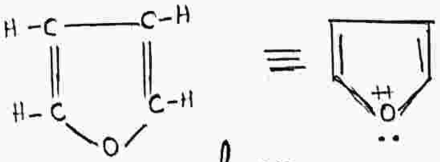
Heterocyclic Compounds (Non - benzenoid aromatic) :

Cyclic compounds in which the ring atoms are made up of hetero atoms like nitrogen, oxygen and sulphur in addition to carbon atoms are called hetrocyclic compounds.

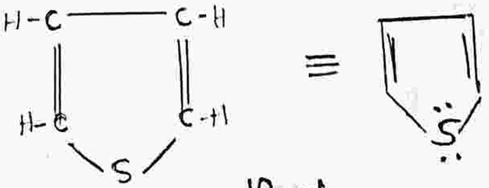
Examples :



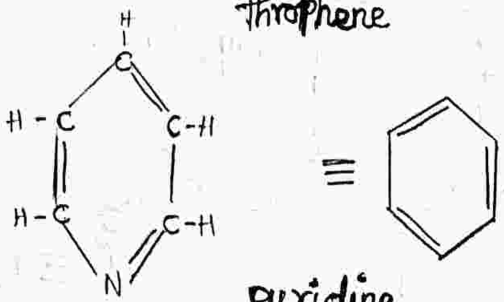
pyrrole



furan



thiophene



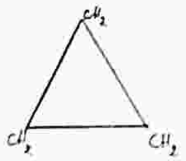
pyridine

The above Compounds are aromatic non-benzenoid Compounds.

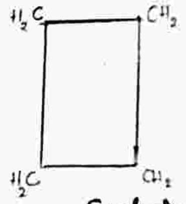
ii, Alicyclic Compounds :

Cyclic Compounds with ring Structure containing only Carbon atoms are called alicyclic or carbocyclic compounds. Though these compounds Prossess a ring Structure, they behave more like aliphatic - Compounds.

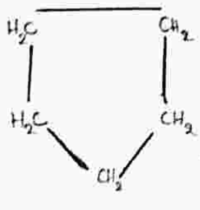
Examples :



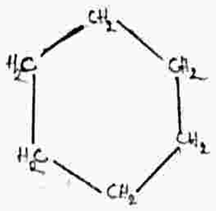
Cyclopropane



Cyclobutane



Cyclopentane



Cyclohexane

The above classification can be Schematically represented as follow:

- Organic Compounds
  - open chain or acyclic compounds
    ethane, propylene, Isobutane
  - closed Chain or cyclic compounds.
    - Homocyclic or Carbocyclic Compounds
      - Aromatic Compounds
        e.g: benzene, toluene, naphthalene, anthracene
        (benzenoides)
      - Alicyclic Compounds
        e.g: cyclopropane, Cyclobutane, cyclopentane, Cyclohexane.
    - Heterocyclic Compounds
      e.g: Pyridine, pyrrole thiophene, furan
      (Aromatic non-benzenoids)

Empirical formula :

Empirical formula of a compound corresponds to its Percentage Composition . It is defined as the ratio of the number of atoms of the different , elements Present in a molecule of the Compound. but it does not give the actual number of atoms of different elements.

For examples , hydrogen Peroxide is made up of hydrogen and oxygen and they are in the ratio of 1 : 1 The empirical formula of hydrogen peroxide is, therefore, HO. But one molecule of hydrogen Peroxide has 2 atoms each of hydrogen and oxygen ie H_2O_2 Thus the empirical formula gives only the ratio and not the actual number of atoms of the different elements Present in a Compound.

Similarly, the empirical formula of glucose is CH_2O indicating that the number of atoms of C, H and O are in the radio of 1:2:1 But we know that one molecule of glucose is made of 6C, 12H and 6O atoms i.e. $C_6H_{12}O_6$ which is not indicated by its empirical formula.

How to arrive at the empirical formula of a Compound?

The Percentage Composition of a Compound is useful in deducing the empirical formula. Following are the different Steps involved.

Step : 1

The percentage of each elements in divided by its atomic weight. Now we get the ratio of the number of atom of each element present in one molecule. This ratio of atoms mostly involves fractions.

Step : 2

a) Since atoms are present in a molecule in the ratio of whole numbers, the fractional ratio obtained in Step 1 Should be reduced to whole number ratio by dividing it by the least number.

b, In Some Cases, Step 2 (a) also does not give whole number ratio. In Such Cases it is necessary either (i) to neglect Very Small fractions or (ii) to multiply the ratio by a Suitable integer to get the whole number ratio.

Step : 3 : The empirical formula, is then arrived at by writing the Symbols of the elements Present along with the above numbers as Subscipts in the lower right Corner.

Problems: The Percentage Composition of glucose is, $C = 39.9\%$, $H = 6.7\%$ and $O = 53.4\%$ Calcute the empirical formula of glucose.

Method 1 :

Step 1 : To obtain the fractional ratio, divide the Percentage of each element by Its atomic weight it by the last number.

b, In Some Cases, Step 2 (a) also does not give whole number ratio. In Such Cases it is necessary either (i) to neglect Very Small fractions or (ii) to multiply the ratio by a Suitable integer to get the whole number ratio.

Step : 3 : The empirical formula, is then arrived at by writing the Symbols of the elements Present along with the above numbers as Subscipts in the lower right Corner.

Problems :

The Percentage Composition of glucose is, $C = 39.9\%$, $H = 6.7\%$ and $O = 53.4\%$ Calcute the empirical formula of glucose.

Method 1 :

Step 1 : To obtain the fractional ratio, divide the Percentage of each element by Its atomic weight

Carbon 39.9/12 = 3.33

Hydrogen 6.7/1 = 6.7

oxygen 53.4/16 = 33.33

The fractional ratio is 3.33 : 6.7 : 33.33

Step 2 : a) To reduce the fractional ratio into the whole number ratio, divided the above ratio by the least number i.e. 3.33

Carbon 3.33/3.33 = 1

Hydrogen 6.7/3.33 = 2.01

oxygen 3.33/3.33 = 1

b, Since the number corresponding to hydrogen has a very small fraction (.01) it is neglected.

So the whole number ratio is 1 : 2 : 1

Step : 3 : Write the empirical formula using the symbols of elements and the above number i.e. $C_1H_2O_1$ or CH_2O

The empirical formula of glucose is CH_2O

Method 2 :
The above calculation can be presented in the form of a tabular column as shown below.

Element	Percentage %	At. Wt	% At. Wt	No in the Previous column / least number?
Carbon	39.9	12	39.9/12 = 3.33	3.33/3.33 = 1
hydrogen	6.7	1	6.7/1 = 6.70	6.70/3.38 = 2.01 to 2
oxygen	53.4	16	53.4/16 = 3.33	3.33/3.33 = 1

∴ Empirical formula of glucose is $C_1H_2O_1$ or CH_2O

Molecular formula :

Molecular formula of a compound corresponds to its molecular weight. It gives the actual number of atoms of the different elements present in a molecule of the compound.

In order to arrive at the molecular formula from empirical formula, the molecular weight of the compound must be known.

a, In the case of a gas, its molecular weight is the weight of the gas that will occupy a Volume of 22.4 litres at N.T.P (i.e. 273 k and 760 mm of pressure).

b, In the Case of liquids and Volatile Solids, the molecular weight is related to Vapour density as shown below.

Molecular weight = 2 × Vapour density

c, In the Case of non- Volatile Substances the molecular weight is determined experimentally by the Conventional methods.

d, In the Case of organic acids and bases, molecular weight Can be Calculated using their equivalent weights.

Molecular weight of an acid = Equivalent weight × Basicity

Molecular weight of a base = Equivalent weight × Acidity

Relationship between empirical formula and molecular formula:

The molecular formula of a Compound may be the Same as the empirical or a Simple multiple of i.e.,

Molecular formula = n× Empirical formula

Where n is an integer. The Same Can also be written as.

n = Molecular formula / Empirical formula

For example, the molecular formula of methane is the Same as its empirical formula CH_4 and the Value of n is 1 in the Case of glucose, the empirical formula is CH_2O and its molecular formula is $C_6H_{12}O_6$. The Value of n is 6

Similarly, the molecular weight of a Compound may be the Same as the empirical formula weight or a Simple multiple of it So equations Similar to the above ones Can be written.

Molecular Weight = n x Empirical formula weight.

n = Molecular weight / Empirical formula weight

Different Compounds may exist for the Same empirical formula But their molecular formulae will be different. Typical examples are ethylene and Propylene. They both have the Same empirical formula i.e., CH_2 but different molecular formulae C_2H_4 and C_3H_6 respectively.

Glucose and acetic acid from another example. Their empirical formula is CH_2O and their molecular formulae are $C_6H_{12}O_6$ and $C_2H_4O_2$ respectively

Examples to Show the Calculation of molecular formula of an organic Compound.

Problems :

1. The empirical formula of glucose is CH_2O. Its molecular weight is 180. Arrive at its molecular formula.

Empirical formula weight = 12+2 +16 = 30

n = Molecular weight / Empirical formula weight

= 180 / 30 = 6

Molecular formula = n × Empirical formula

= $6 \times CH_2O$ i.e., $C_6H_{12}O_6$

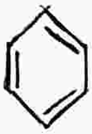
Resonance Concept :

A number of organic Compounds cannot be accurately represented by one Structure. For example, benzene is ordinarily represented as:

This Structure has three carbon - Carbon single bonds and three carbon - Carbon double bonds. However, it has been determined experimentally that all carbon - Carbon bonds in benzene are identical and have the Same bond length (1.39 Å). Further more, the Carbon - Carbon bond length of (1.39 Å) is intermediate.

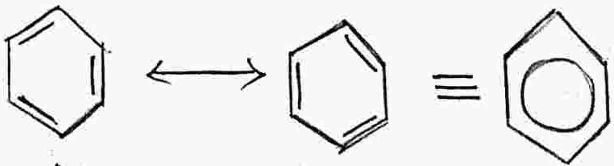
between the normal Carbon - Carbon double - bond length (1.34 Å) and the normal carbon - carbon single - bond length (1.54 Å). Actually two alternative structure (1 and 2) can be written for benzene :

1



2

These two structure differ only in the position of electrons. Neither (1) nor (2) is a correct representation of benzene. The actural structure of benzene lies some where between these two structure. This phenomenon in which two or more structure can be written for a compound which involve identical positions of atoms is called Resonance.



1 2 3

Benzene Benzene

The actual Structure of the molecule is Said to be a Resonance Hybrid of Various Possible alternative Structure. The alternative. Structure are referred to as the Resonance Structure or Canonical forms. A double headed arrow(⟺) between the resonance Structure is used to represent the resonance hybrid. Thus in the Case of benezene, (1) and (2) represent the resonance Structures. Actual Structure of the molecule may be represented as hybrid of these two resonane Structure, or by the Single Structural formula (3).

It Should be clearly understood that the resonance Structures (1) and (2) are not actual Structure of the benzene molecule. They exist only in theory. None of these Structure adequately represents the molecule. In resonance theory, we View like benzene molecule Which is of Course a real entity an being hybrid of these two hypothetical resonance Structure.

A green mark Produced by OverPrinting blue with yellow is a good Visual analogy to the resonance Concept. Yellow and blue Correspond to the resonance Structure (Canonical forms) and the green Corresponds to the hybrid Structure.

The resonance hybrid is more Stable than any one of the Various resonance Structure. The different in energy between the hybrid and the most Stable resonance Structure is known as the Resonance Energy. Resonance energy Can be determined by the difference between the calculated and experimental heats of combustion (energy given off as heat when one mole of Compound is burned) of the Compound. For example, it has been Calculated that the hypothetical Structure (1) or (2) would have a heat of Combustion of 797 kcal/mol. The measured Value for the heat of Combustion of benzene is 759 kcal/mol. Therefore, the resonance energy of benzen is (797-759) kcal/mol or 38 kcal/mol.

The benzene is said to be "Stabilized" by a resonance energy of 38 kcal/mol (Fig. 5.40)

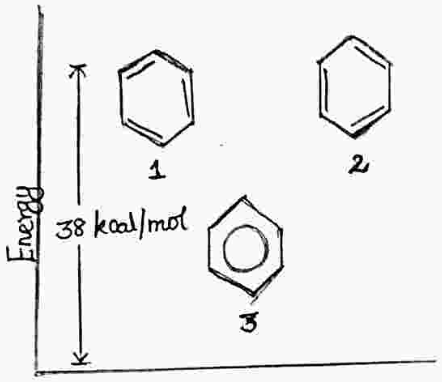
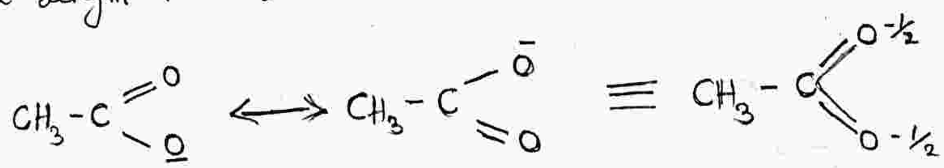


Fig. 5.40. Resonance energy of benzene

Another Species that is not correctly represented by a Single Sturucture is the acetate ion. As in the case of benzene, acetate ion is a hybrid of two resonance Structure. Both carbon - oxygen bonds in the acetate ion are identical and have the Same bond length (1.26Å). The Carbon - oxygen bond length of 1.26Å is intermediate between the normal Carbon - oxygen double - bond length (1.20Å) and the normal carbon - oxygen Single bond length (1.43Å)



$$CH_3-C(=O)\underline{O}^- \longleftrightarrow CH_3-C(\bar{O})=O \equiv CH_3-C(O^{-1/2})(O^{-1/2})$$

Acetate ion   Acetate ion

Rules Governing Resonance :-

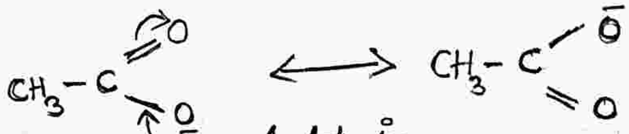
The resonance Concept is extremely useful in organic chemistry, and will come up a number of times. The following are some important rules governing resonance.

(1) Resonance occurs whenever a molecule can be represented by two or more structure differing only in the arrangement of electrons. Without shifting any atoms. Resonance only involves the delocalization of electrons.

(2) Resonance structure are not actural structure for the molecule. They are nonexistent and hypothetical.

(3) Resonance structure are interconvertible by one or a series of short electrons -Shifts. for examples.

Benzene



Acetate ion

(4) Resonance hybrid represents the actual Structure of the molecule. The Structure of the resonance hybrid is intermediate between the Various resonance Structure and is not a mixture of them. (5) The Resonance hybrid is represented by a double headed arrow (↔). This Should not be Confused with the two arrows. (⇄) used to denote equillbruim between two different Compounds.

(6) Resonance hybrid is more Stable than any of its Contributing forms (resonance Structure)

(7) Resonance always increases the Stability of a molecule ond lessens its reactivity

In a Chemical reaction, the reactant molecule undergoing attack is referred to as the Substrate and the general term used to describe the attacking Species is the **Reagent**. The Substrate and the reagent Interact to yield the Products of the reaction.

Substrate + Reagent → Products

The Carbon bonds in the Substract molecule are broken (or cleaved) to give fragments which are very reactive and Constitute transitory intermediates. At once they may react with other Species Present in the environment to form new bonds to give the Products

The Steps of an organic reaction Showing the breaking and making of new bonds of Carbon atoms in the Substrate leading to the formation of the final Products through transitory intermediates, are often referred to as its Mechanism

Substrate → Intermediate (transitory) → Products

Most of the attacking reagents Carry either a positive or negative charge. The positively Charged reagents attack the regions of high electron density in the Substrate molecule. on the other hand, the negatively charged regents will attack the regions of low electron density in the Substrate molecule.

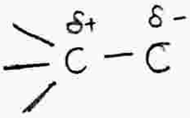
Factors which Influence a Reaction :

A reaction may occurs or may not occur depending upon the density of electrons at the side of reaction in the Substrate. The factors which influence the electron density in the Substrate are :

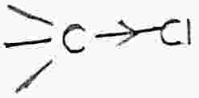
(1) Inductive Effect
(2) Mesomeric Effect
(3) Electromeric Effect

Inductive Effect : It involves σ electrons. The σ electrons which form a Covalent bond are Seldom shared equally between the two atoms. This is because different atoms have different electronegativity Values, i.e., different Powers of attracting the electrons in the bond. Consequently, electrons are displaced towards the more electronegative atom. This introduces a Certain degree of polarity in the bond. The more electronegative atom acquires a small negative charge (δ_-). The less electronegative atom acquires a small positive charge (δ_+).

Consider the Carbon - chlorine bond. As Chlorine is more electronegative, it will become negatively charged with respect to the carbon atom.



1



2

3

Structure (1) indicates the relative charges on two atoms. In (2), the arrow head placed in the middle of the bond indicates the direction in which the electrons are drawn. In (3), the more heavily shaded part shows the region in which the electron density is greatest.

The inductive effect (I Effect) refers to the polarity in a molecule as a result of higher electronegativity of an atom Compared to another :

The Carbon – hydrogen bond is used as a Standard. Zero-effect is assumed in this case. Atoms or groups which lose electrons toward a Carbon atom are Said to have a +I Effect. Such groups will be referred to in this book as electron-releasing. Those atoms or groups which draw electrons away from a Carbon atom are Said to have a -I Effect. Such groups will be referred to as electron-attracting

Some Common atoms or groups which Cause +I or -I Effects are shown below:

(a) -I Effect Groups (Electron-attracting)

NO_2, F, Cl, Br, I, OH, $C_6H_5^-$

(b) +I Effect Groups (Electron-releasing)

$(CH_3)_3C^-$, $(CH_3)_2CH^-$, $CH_3CH_2^-$, CH_3^-

Tertiary alkyl groups exert greather +I effect than Secondary which in turn exert a greather effect than Primary.

An inductive effect is not Confinued to the Polarization of one bond. It is transmitted along a chain of Carbon atoms, although it tends to be insignificant beyond the Second Carbon.

$$-\underset{3}{C} - \underset{2}{C} \rightarrow \underset{1}{C} \twoheadrightarrow \underset{-1}{Cl}$$

The inductive effect of C_1 upon C_2 is Significantly less than the effact of the Chlorine atom on C_1.

The inductive effect results in a Permanent State of the molecule and Can be observed Practially in the from of dipole moments. The effect does not depend upon the presence of a reagent.

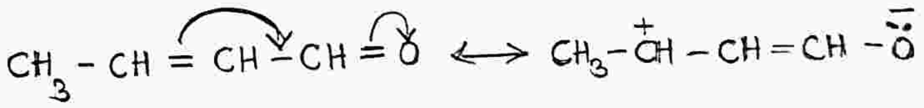
Mesomeric Effect : It involves π electrons of double and triple bonds.

The Mesomeric effect (M effect) refers to the polarity Produced in a molecule as a result of interaction between two π bonds or a π bond and lone Pair of electrons. The effect is transmitted along a chain in a similar way as are inductive effects.

The mesomeric effect is of great importance in Conjugated compounds. (Conjugated compounds are those in which the Carbon atoms are linked alternately by single and double bonds) In Such Systems, the π electrons get delocalized as a Consequence of mesomeric effect, giving a number of resonance Structures of the molecule.

Consider a Carbonyl group ($>C=O$). The oxygen atom is more electronegative that the Carbon atom. As a result, the π electrons of the Carbon-oxygen double bond get displaced toward the oxygen atom. This gives the following resonance Structure.

The mesomeric effect is represented by a Curved arrow. The head of the arrow indicates the movement of Pair of π electrons. It the Carbonyl group is conjugated with a Carbon - Carbon double bond, the above Polarization will be transmitted further via the π electrons.



$CH_3-CH=CH-CH=O \longleftrightarrow CH_3-\overset{+}{C}H-CH=CH-\bar{\ddot{O}}$

The mesomeric effect like the inductive effect may be Positive or negative. Atoms which lose electrons toward a Carbon are Said to have a +M Effect. Those atoms or groups which draw electrons away from a Carbon atom are Said to have a -M effect.

Some Common atoms or groups which Cause +M or -M effects are listed below.

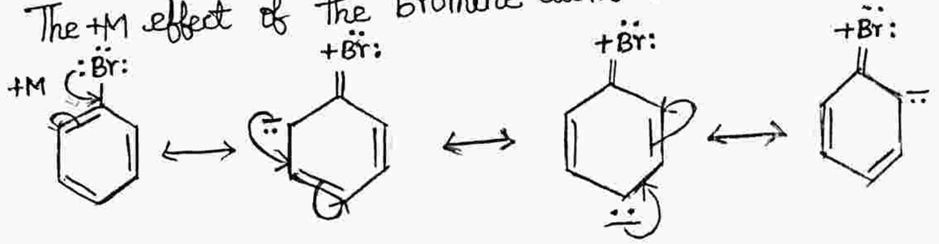
(a) +M effect Groups

Cl, Br, I, NH_2, NR_2, OH, OCH_3

(b) -M Effect Groups :

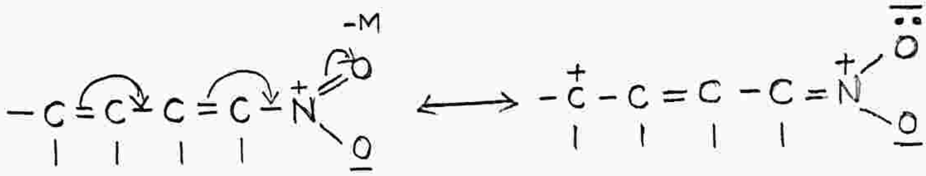
NO_2, CN > C = O

The +M effect of the bromine atom is shown below :



Bromobenzene

The -M effect of the nitro group is shown below:



$$-\underset{|}{C}=\underset{|}{C}-\underset{|}{C}=\underset{|}{C}-\overset{+}{N}{\overset{\displaystyle =O}{\underset{\displaystyle \underline{O}}{}}} \longleftrightarrow -\underset{|}{\overset{+}{C}}-\underset{|}{C}=\underset{|}{C}-\underset{|}{C}=\overset{+}{N}{\overset{\displaystyle \bar{O}}{\underset{\displaystyle \underline{O}}{}}}$$

The mesomeric effect like the inductive effect result in a Permanent State of the molecule. It does not depend upon the Presence of reagent.

The inductive and mesomeric effects indicate the charge distribution in a molecule. Thus they provide an effective way of determining the point of attack of electrophiles and nucleophiles on the molecule.

Electromeric Effect: Like the mesomeric effect, it also involves the π electrons.

The electromeric effect (E Effect) refers to the polarity Produced in a multiple bonded Compound as it is approached by a reagent.

When a double or a triple bond is exposed to an attack by an electrophile E^+ (a reagent) the two π electrons which from the π bond are Completely transferred to one atom or the other. The electromeric effect is represented as:

$$A \overset{\frown}{=} B \xrightarrow[\text{Reagent}]{E^+} \overset{+}{A} - \overset{-}{\ddot{B}}$$

The Curved arrow Shows the displacement of the electron Pair. The atoms A has lot is Share in the electron Pair and B has gained this Share. As result, A acquires a Positive Charge and B a negative Charge. Notice that the arrow points away from the centre of the bond and towards the atom that gains the electron pair.

Consider the example where an elecrophile (E^+) attacks a Carbon - Carbon double bond in the ethylene molecule. We know that the double bond is made up of one σ bond and one π bond. The electrons in the π bond are quite exposed. Under the influence of the electric field of the positively Charged electrophile, the Symmetry of the molecular orbital is distubed entirely in favor of one carbon atoms as Shown in Fig. 6.1

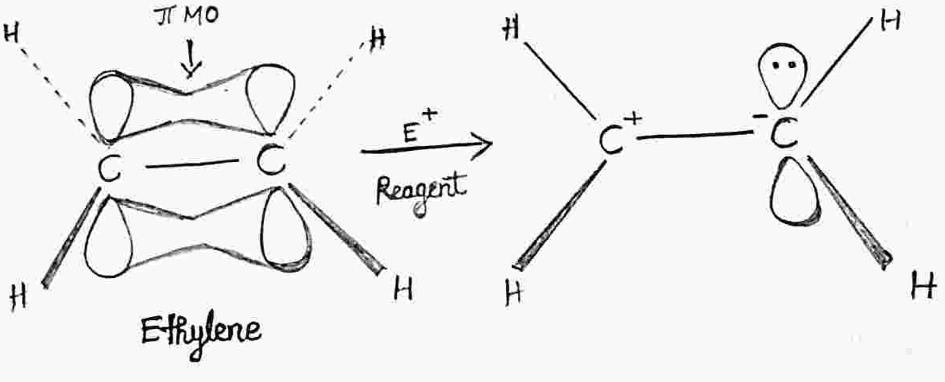


Fig. 6.1. The presence of an electrophile disturbs the Symmetry of the π MO in favor of one of the carbon atoms in ethylene.

This gives a negative charge to the carbon atom to which the π electron-pair migrates, while the other atom acquires a possitive Charge.

$\mathrm{H-\underset{H}{\underset{|}{C}}\equiv\underset{H}{\underset{|}{\overset{\curvearrowright}{C}}}-H\xrightarrow{E^{+}}H-\underset{H}{\underset{|}{\overset{+}{C}}}-\underset{H}{\underset{|}{\overset{\cdot\cdot\,-}{C}}}-H}$

The electromeric effect is a temporary effect. It takes Place only in the Presence of a reagent.

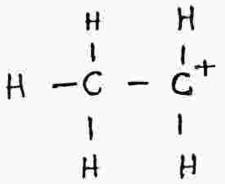
HyperConjugation :

The relative Stability of Various classes of Carbonium ions may be explained by number of no-bond resonance Structure that Can be written for them. Such Structure are arrived at by Shifting the bonding electrons from an adjacent C-H bond to the electron-deficient Carbon. In this way, the Positive Charge originally on carbon is dispersed to the hydrogen. This manner of electron release by assuming no-bond character in the adjacent

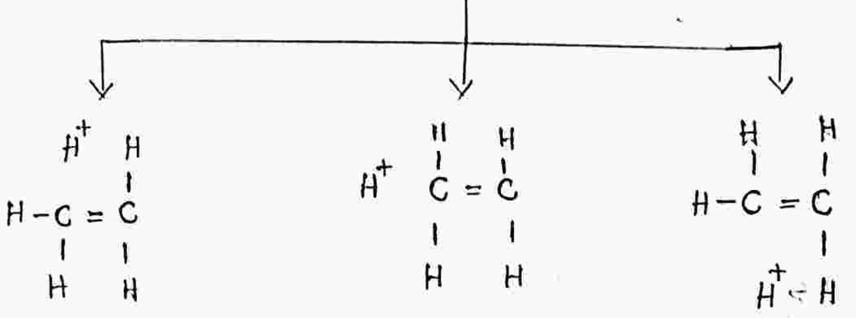
C-H bond is called Hyper Conjugation or No-Bond Resonance

The more hyper Conjugation Structure (no-bond resonance Structure) that can be written for a Species, the more Stable is the Species. For examples,

(1) Ethyl Carbonium ion is Stabilized by three hyperConjugation Structure :



Ethyl carbonium ion



(2) IsoProply Carbonium ion is Stabilized by six hyper Conjugation Structure.

(3) t-Butyl Carbonium ion is Stabilized by nine hyper Conjugation Structure. Thus, the following order of stability holds :

$$(CH_3)_3\overset{+}{C} > (CH_3)_2\overset{+}{C}H > CH_3\overset{+}{C}H_2 > \overset{+}{C}H_3$$

In general resonance effects (mesomeric effects) are more important than hyperconjugation effects. The allyl and benzyl Carbonium ions are more Stable than most alkyl Carbonium ions because the former are Stabilized by resonance while the latter are Stabilized by hyperconjugation.

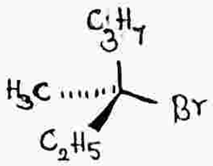
Steric effects :

When two (or) more groups (or) atoms Come in Close Proximity to each other Precisely within each other's Vander Walls radii and result in a meeheal replusiion. This mater molecule unstable.

When two atoms get to close, into each other's Vander walls's radii, the electron cloud Surrounding each atom repal each other leading to a lot of distabillisation.

Steric effect affeels different properties of molecules like acidity barisity & general reactivity

A Substitution reaction on a holide by a hydroxides does not work in this care because of steric hindrance.



+ Koll ⟶ No Reaction

due to Steric effect.

So Sterics can help us rule out certain reaction mechanism and help us predict the reactivity of cerbin molecules in certain reaction.

unit - 4

①

Classification of physical properties of materials

① Intensive and extensive physical properties :

physical properties may be classified as either intensive (or) Extensive. Intensive physical properties do not depend on the sample's size (or) mass. Examples of intensive properties include boiling point State of matter and denity. Extensive physical properties depend on the amount of matter in the sample Examples of extensive properties include size. Mass and Volume.

2) Additive properties.

When a property of a substance is equal to the sum of the corresponding properties of the constituent atoms, it is called an additive property eg) molecular mass of a compound is given by the Sum of the atomic masses of the constituent atoms

③ Constitutive Property :

A property that depends an the arrangement of atoms and bond structure in a molecule, is refered for as a constifutive property surface tension and viscocity and optical activity are example of constitutive property.

Additive and Constitutive property :

An additive property which also depends on the intra molecular structure called additive and constitutive property surface tension and viscosity are such properties

Surface tension and chemical Constitution parachors.

From a study of a large number of liquid

$$\frac{\gamma^{1/4}}{D-d} = c \quad —— ①$$

γ → surface tension
D → Density
d → density of vapour at the same temperature
c → constant.

Modified this equation by multiplying both sides by M. the molecular weight of the liquid

$$\frac{M\gamma^{1/4}}{D-d} = Mc = [P] \quad —— ②$$

The quantity [P], which was constant for a liquid, was gives the name paracha, As d is negligible compared to D the equation (2) reduces to

$$\frac{M}{D}\gamma^{1/4} = [P]$$

$$\text{(or)} \quad V_m \gamma^{1/4} = [P] \quad —— ③$$

Where V_m is the molar volume of the liquid. If surface tension (γ) is unity, from eq(03) we may write

$$[P] = V_m$$

Thus the parachor [P] may be defined as the Molar volume of a liquid at a temperatures so that its surface tension is unity

uses of parachors in elucidating structure :-

The experimental parachor valumes of several organic compounds of known molecular structure. The parachor is both an additive and constitutive property. That is the parachor of an individual compound can be expressed as a sum of.

① Atomic parachors :-

Which are the contribution of each of each of the atoms present in the molecule.

② structural parachors:-

Which are the contributions of the various bonds and rings present is the molecule.

By correlating the experimental values of parachors with molecular structure. Sugden (1924) calculated the atomic and structural parachors listed in Table.

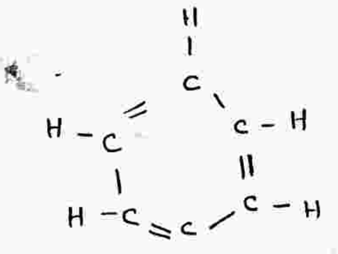
Some atomic and structural parachor's.

Atom	Parachor's Singular	Parachor's Vegel	Bond (or) Ring	Parachors Singular	Parachors Vegal
C	4.8	8.6	Single bond	0	0
H	17.1	15.7	Double	23.2	19.9
O	20.0	19.8.	coordinate	1.6	0
N	12.5	-	5 membered ring	17.0	12.3
Cl	54.3	55.2	6 - membered ring	6.1	1.9.

parachors Studies in the elucidation of molecules structure :-

① Structure of benzene (vogel)

If the kekule formula for benzene be accepted the value of its paracha can be calculated by using vogal's



Kekule formula

6c 6 × 8.6 = 51.6

6H 6 × 15.7 = 94.2

3(=) 3 × 19.9 = 59.7

6 - membered ring = 1.4

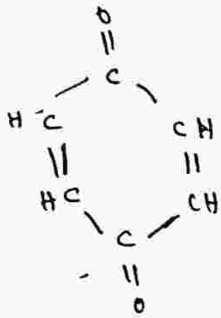
parachor of benze = 206.9

The experimental value of the parachor of benzene is 206. 9. since the calculated parachor.

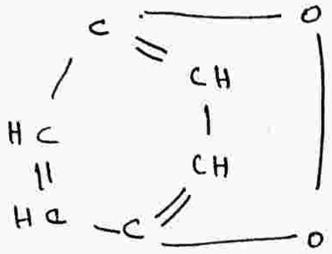
with that determind by experiment the kekule structure for benzene is supported

② structure of Quinone (sugden)

The two possible structural formulas proposed for quinone are



(A)



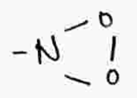
The parachors calculated for the two Structures are

	Structure – A		Structure – B
6C	6 × 4.8 = 28.8	6C	6 × 4.8 = 28.8
4H	4 × 17.1 = 68.4	4H	4 × 17.1 = 68.4
2O	2 × 20.0 = 40.0	2O	2 × 20.0 = 40.0
4 (=)	4 × 23.2 = 92.8	3 (=)	3 × 23.2 = 69.6
1-six-membered ring	1 × 6.1 = 6.1	2-sixmembered rings	2 × 6.1 = 12.2
	Total = 236.1		Total = 219.0

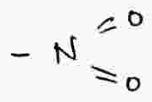
The experimental value of parachors for quinone is 236.8 This corresponds to the parachor Calculated from structure. A therefore the structure A represents quinone correctly.

③ structure of Nitro group (sugden).

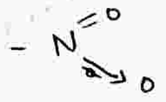
The parachor has also been found usefull in providing information regarding the nature of bonds present in certain groups. The nitro group ($-NO_2$) for ⑥ example. may be represented in three ways



I



II



III

The calculated parachore are

Structure I		
1N	1 × 12.5 = 12.5	
2O	2 × 20.0 = 40.0	
3. m	1 × 17.0 = 17.0	
	Total	= 69.5

Structure II		
1N	1 × 12.5 = 12.5	
2O	2 × 20.0 = 40.0	
2(=)	2 × 23.2 = 46.4	
	Total	= 98.4

Structure II		
1N	1 × 12.5 = 12.5	
2O	2 × 20.0 = 40.0	
1(→)	1 × (−1.6) = −1.6	
	Total	= 74.1

The exprimental value of parachor for $-NO_2$ group has been found to be 73.0 this approximates to the calculated parachor for structure III which is therefore the appropriate structure of $-NO_2$ group

Rheochor :-

If molecular volume (m/d) be multiplied by the eighth root of the coefficient of viscosity it gives a constant value [R]. The quantity [R] is termed Rheochor

$$\frac{M}{d} \times \eta^{1/8} = [R]$$

The Rheochor may be defined as the molar volume of the liquid at the temperature at which its viscosity is unity like parachor rheachor is both additive and constitutive.

However it has not proved of much use in solving structural preplems.

Bond moment :-

Any bond which has a degree of polarity has a dipole moment. this is called Bond moment The dipole moment of H-H bond is zero because it is nonpolar. The dipole moment of the H-Cl bond is 1.08 D because it is polar. In a diatomic moleculat, the bond moment corresponds to the dipole moment of the molecule The dipole moments of the halogen halides show , below also indicate their bond moments.

Their bond moments indicate

$$\underset{H \longrightarrow F}{\overset{1.91\,D}{+\!\!\longrightarrow}} \qquad \underset{H \longrightarrow Cl}{\overset{1.08\,D}{+\!\!\longrightarrow}} \qquad \underset{H \longrightarrow Br}{\overset{1.80\,D}{+\!\!\longrightarrow}} \qquad \underset{H \longrightarrow I}{\overset{0.42\,D}{+\!\!\longrightarrow}}$$

The bond moment decreases with decreasing electronegati of the halogen atom. when a molecule contains three (or) more atoms each bond has a dipole moment p for example.

$$\underset{C \longrightarrow H}{\overset{0.4\,D}{+\!\!\longrightarrow}} \qquad \underset{C \longrightarrow Cl}{\overset{1.5\,D}{+\!\!\longrightarrow}} \qquad \underset{H \longrightarrow O}{\overset{1.5\,D}{+\!\!\longrightarrow}} \qquad \underset{H \longrightarrow N}{\overset{1.3\,D}{+\!\!\longrightarrow}}$$

The net dipole moment of the molecule is the vector resulted of all the individual bond moment If a molecules is symmetrical having identical bonds its dipole moment is zero. That is so because the individual bond moments cancel each other out

Dipole moment and Ionic character :-

The magnitude of the dipole moment of a diatomic molecule determines its ionic character let us consider an HBr molecule whose measured dipole moment (μ_{exp}) is 0.79 D and bond distance $(r) = 1.41 \mathring{A}$ If the molecule were completely Ionic $(H^+ Br^-)$ each of the ions will bear a unit electronic charge e $(4.8 \times 10^{-10}$ esu). Thus the dipole moment of the ionic molecules (μ_{ionic}) can be calculated

$$\mu_{ionic} = e \times r = (4.8 \times 10^{-10} \text{ esu})(1.41 \times 10^{-8} \text{ cm})$$

$$= 6.77 D$$

But the experimental dipole moment (μ_{exp}) of $H^{\delta+} - Br^{\delta-}$ which determines its actual fractional ionic character is 0.79 D Therefore

$$\% \text{ ionic character of HBr} = \frac{\mu_{expt}}{\mu_{ionic}} \times 100$$

$$= \frac{0.79 D}{6.77 D} \times 100$$

$$= 11.6$$

Hence HBr is 12% ionic in Character.

~~Colligative property :-~~

Colligative property :-

The properties which depend on the number of particles in the Solution and not on their nature are called colligative properties

eg) vapour pressure elevation in boiling point depression in freezing point

Scalar and vector properties

⑨

physical quantities

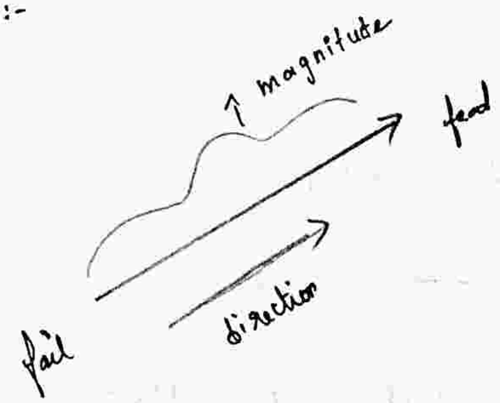
scalar
(has magnitude only)

vector
(has magnitude and direction)

Scalars :-

scalar quantities are those quantities complete specifications. physical quantities which can be completely specified by a number and unit and therefore have the magnitude only are scalars
Some physical quantities which are scalar are mass, length, time, energy, volume, denity, temperature, electric, charge, electric potential These examples obey the alge braic

Vectors :-



vector quantities are those quantities which require magnitude as well as direction for their complete specifications vectors are physical quantities, which besides having both magnitude and direction also obey the law of geometrical addition (The law of geometrical) addition (i-x) the law of trianqular addition and law of parellilogram are discussed later in this chapter) Some physical quantities, which are vectors are displacement, velocity, acceleration, force, electric intensity, magnetic, intensity, acceleration, force, electric magnetic moment etc. vector quantities cannot in general be added is algebraically

Electric current prossesses magnitude and direction (through the conductor) but it is not a vector quantity. Electric current is a scales quantity.

M = molecular weight.

ρ = density

paramagnetic susceptibility χ_m may be related to permanent magnetic moment μ_m by the relation

$$\chi_m = \frac{N_A \cdot \mu_m^2}{3kT} + N_A \alpha_m \quad \text{——} ③$$

Where N_A : Avagadro number k = Boltzmann constant

T = Absolute temperature

α_m = magnetic polarization (constant)

2.12 Diamagnetism, paramagnetism, ferromagnetism Antiferro and ferrimagnetism

i) Diamagnetism.

Substances which repel the magnetic lines of forces are called diamagnetic and the property is termed as diamagnetism. In a diamagnetic substance all the electron spins are paired. Diamagnetic substance donot have a permanent magnetic moment.

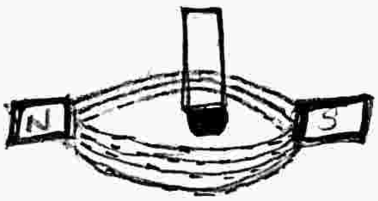
examples :- Sb, Bi, Zn, Ag, Au, Pb. etc

Charecteristics:-

i) magnetic permeability is < 1

ii) magnetic susceptibility is negative and independent of temperature

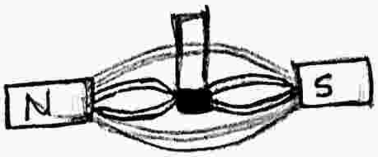
iii) In an external magnetic field. they get magnetised in a direction opposite too the field. Hence diamagnetic is a substances have a tendency to move away from field (stronger to weaker field)



ii) paramagnetism:-

Substances which attract the magnetic lines of forces are called paramagnetic. and the property is termed as paramagnetism. paramagnetism arises from the net spin angular momentum and orbital angular momentum of the unpaired electrons. They align parallel to the field. paramagnetism is inversely proportional to temperature

examples O_2, NO, salts of Cr, Mn, Ni etc.



characteristics :-

- * magnetic permeability is > 1
- * magnetic susceptibility is positive and decreases with rise in temperature
- * In an external magnetic field, they get magnetised in the direction of the field.
- * They move from weaker to stronger part of the external field.

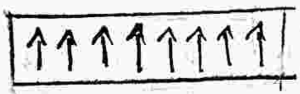
iii) Ferro magnetism :-

substances which are highly paramagnetic and retain magnetic property when removed from the magnetic field are ferromagnetic. In ferromagnetism the moments on direction. they are strongly magnetised. molar magnetic susceptibility is very high. Ferromagnetism depends on temperature and field strength

examples :- Iron, Cobalt and Nickel.

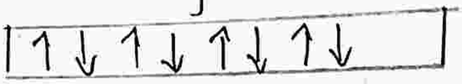
Characteristics :

- * magnetic permeability is very high ($\mu >> > 1$)
- * magnetic susceptibility is very large
- * In an external magnetic field, they are strongly magnetised
- * As temperature increases magnetic susceptibility decreases Above a temperature called curie temperature, ferro magnetism becomes paramagnetism.



IV. Antiferro magnetism :

In antiferro magnetism, co-operative effects (allignment of Individual moments) leads to alternating spin orientantions. The dipoles have equal moments. but adjacent dipoles point in opposite direction. This leads to low magnetisation. examples :- $KNiF_3$, MnO, $K_2O_8Cl_6$ Anti ferromagnetisation transitions occur at the Neel temperature. Above Nell temperature they behave as simple paramagnetic



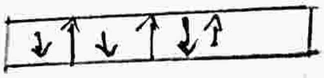
(Alignment of magnetic moments in antiferromagnets)

V) Ferri magnetism :-

In ferri magnetic materials (ferrites) the magnetic moment of adjacent ions are antiparallel and of unequal strength. Hence there is a finite net magnetism. The resultant net magnetism lies in between ferro magnetism and antiferromagnetism.

example :- $MnFe_2O_4$

moreover, when the temperature is above a critical value, the material becomes paramagnetic.



2.13 The electron theory of magnetism

i) Explanation of diamagnetism :-

Diamagnetism is associated with atoms containing an even number of electrons. Therefore in a dia magnetic substance all the electron spin are paired. The electron in each pair have orbital motions as well as spin motions in opposite sense. The resultant magnetic moment of the atom is thus zero. When such a substance is placed in a magnetic field. the field does not lend to align the atoms acquire an effective magnetic dipole moment which is opposite to the applied field. Hence diamagnetic susceptibility is negative and very small.

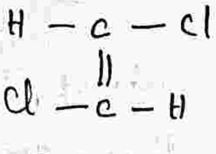
ii) Explanation of paramagnetism:-

In paramagnetic materials, the magnetic fields associated with orbital and spinning electrons do not cancel out. there is a net intrinsic moment in it. The molecules in it behaves like little magnets. When such a substances is placed in a external magnetic field, it will align parallel to the external magnetic field. It tends to more further into the field. there is force of attraction. the molar magnetic susceptibility is positive. when a paramagnetic substance is heated the thermal motion of a atoms increases and the alignment of the dipoles become more difficult. Hence paramagnetic susceptibility decreases with rise temperature.

$$Z_m \propto = \frac{1}{T}$$

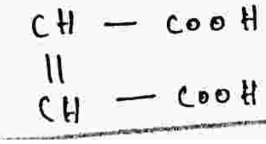
$$\begin{array}{l} H - C - Cl \\ \quad \| \\ H - C - Cl \end{array}$$

cis - Dichloroethene
(μ = 1.85 D)



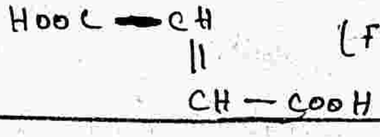
$$\begin{array}{l} H - C - Cl \\ \quad\ \| \\ Cl - C - H \end{array}$$

Trans - Dichloroethene
(μ = 0)



$$\begin{array}{l} CH - COOH \\ \| \\ CH - COOH \end{array}$$

maleic acid
(cis)
(μ = 3.17 D)

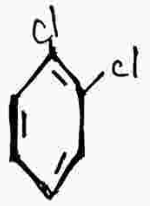


$$\begin{array}{l} HOOC - CH \\ \qquad\quad \| \\ \qquad\quad CH - COOH \end{array}$$

(Fumaric acid)
(trans)
(μ = 2.46 D)

ix) ortho, meta and para isomers :-

The dipole moment values are quite informative in distinguishing between ortho, meta and para derivatives of benzene. If the two substance are identical, the symmetrical para isomer will have no dipole moment while the ortho and meta isomers possess appreciable dipole moments.



o - Dichlorobenzene
(μ = 2.598 D)

m - Dichlorobenzene
(μ = 1.5 D)

p - Dichlorobenzene
(μ = 0)

MAGNETIC PROPERTIES

1) magnetic susceptibility

When a substance is placed in a magnetic field it gets magnetised. This means that magnetic moments is induced in its molecules. This is known as induced magnetisation. The magnetic moment induced per unit volume of the substance is called the intensity of magnestisation. If M is the intensity of magnetisation. and H is strength of the magnetic field then the ratio M/H is called magnetic susceptibility, k

$$k = \frac{M}{H}$$

The magnetic susceptibility divided by density is termed the specific magnetic susceptibility.

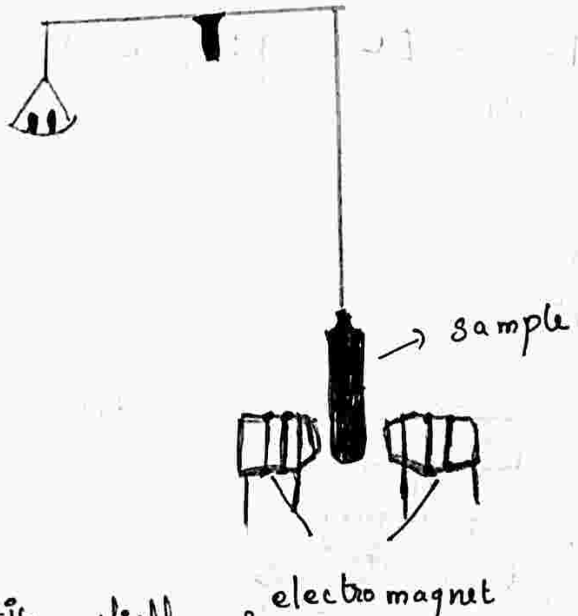
$$\chi = \frac{K}{\rho}$$

The specific magnetic susceptibility multiplied by the molecular weight of the substance is known as molar magnetic susceptibility.

$$\chi_m = \chi . H$$

Determination of magnetic susceptibility by Gouy's method:

The specific magnetic susceptibility, χ of a substance can be readily measured with a magnetic balance called Gouy's balance. A cylindrical tube is counter balanced by placing weight in the pan attached to the other arm of the balance. cylindrical tube containing the sample is suspended from one arm of the balance between the two poles of an electromagnet.



When the magnetic field is switched on, the sample experiences a change in mass. Δm. it is related to the magnetic susceptibility through the equation

$$\Delta m . g = \frac{1}{2} (\rho\chi - \rho_0 \chi_0) A H^2$$

(or)

$$\Delta m \propto (\rho\chi - \rho_0 \chi_0) \text{ at constant } A \text{ and } H$$

where A = Area of cross section of the sample tube.

The experiment is repeated with a sample of known magnetic susceptibility, usually water in the same magnetic field. Then.

$$\frac{\Delta m}{\Delta m_s} = \frac{\rho\chi - \rho_0 \chi_0}{\rho\chi_s - \rho_0 \chi_0}$$

where.

Δm = Charge in mass of the sample

ρ = Density of the sample

Δm_s = charge in mass of water

ρ_s = Density of water

ρ_0 = Density of air

χ_0 = Specific magnetic susceptibility of air

χ_s = Specific magnetic susceptibility of water.

2. Magnetic moment :

An electron in motion (orbital motion or spin) behaves like a small magnet and produces a magnetic field called magnetic moment. paramagnetic substances possess a net magnetic moment due to the presentence of one or more unpaired electrons. In diamagnetic substances the electrons are paired and the magnetic moments get concelled.

Determination of magnetic moment :

The magnetic moments of paramagnetic substances may be calculated from their magnetic susceptibilities using Langevin

$$\chi_m = \frac{\mu_m{}^2 N}{3kT}$$

where. μ_m = magnetic moment in BM
N = Avogadro number
k = Boltzmann Constant

Application of magnetic moment :-

magnetic moments are used to determine the number of unpaired electrons in odd electron molecule free radicals and ions. The magnetic moment is related to the number of electrons by the expression

$$\mu_m = \sqrt{n(n+2)}$$

magnetic moments are expressed in Bohr magneton (BM)

$$1BM = 9.273 \times 10^{-24} JT^{-1}$$ (Joule per tesla)

Illustration :-

1. $TiCl_3$ ($3d^1$ configuration) has 1 unpaired electron and has a magnetic moment of 1.73 B.M. its calculated magnetic moment will be

$$\mu_m = \sqrt{n(n+2)}$$
$$= \sqrt{1(1+2)}$$
$$= \sqrt{3}$$
$$= 1.732 \text{ BM}$$

2. $FeCl_3$ ($3d^5$ configuration) has 5 unpaired electrons

$$\mu_m = \sqrt{n(n+2)}$$
$$= \sqrt{5(5+2)}$$
$$= \sqrt{5(7)}$$
$$= \sqrt{35}$$
$$= 5.91 \text{ BM}$$

2:14 Measurement of magnetic susceptibility using Gouy's balance :-

magnetic susceptibility is measured using Gouys balance. The sample is taken in a cylindrical tube which is suspended vertically between the poles of a strong electromagnet (by means of a wire from one arm of the balance) when the electromagnet is turned on, a paramagnetic substance is pulled by the magnetic field and weights are added to counter balance the force. on the other hand, a diamagnetic substance is repelled by the magnetic force acting on the material. If Δm is the additional weight to be added (or substracted)

then $\Delta m.g = \frac{1}{2} A H^2 (\rho\chi - \rho_0 \chi_0)$

A = Area of cross section of the sample tube.

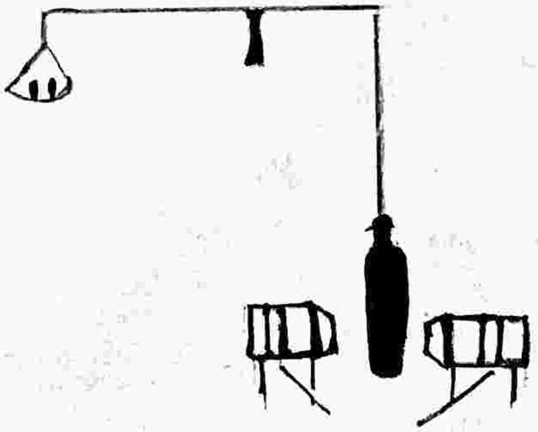
H = Field strength

ρ = Density of the sample.

ρ_0 = Density of air

χ = magnetic susceptibility

g = Acceleration due to gravity.



Gouys method for measurement of magnetic susceptibilities.

χ_0 = magnetic susceptibility of air

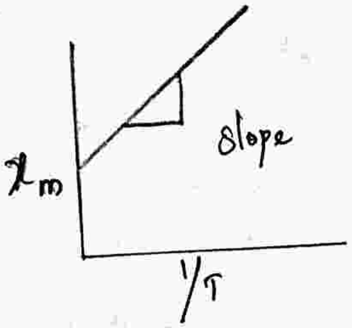
Thus the magnetic susceptibility (χ) of the sample is determined. In the above calculations, the absolute value of the field strength H is required. However measurement of H and A can be eliminated if the experiment is first performed with a substance of known magnetic susceptibility. using the same magnetic field and the same cylinderical tube.

2.15 Determination of magnetic moment of paramagnetic substance (μ_m)

The molar magnetic susceptibility (χ_m) a paramagnetic substance is related to its magnetic moment μ_m by the relation

$$\chi_m = \frac{N_A \cdot \mu_m^2}{3KT} + N_A \alpha_m \qquad \text{---} ①$$

α_m = constant
N_A = Avagadro number
k = Boltzman constant.
T = Absolute temperature



A plot of χ_m against 1/T would give a straight line with slope

Value equal to $\frac{N_A \cdot \mu_m^2}{3k}$

from the slope value μ_m can be calculated

$$\mu_m = \sqrt{\frac{3k\,\text{slope}}{N_A}}$$

2.16 Relationship between magnetic moment and number of unpaired electron :-

The total magnetic moment of any substance is the sum of orbital motion and spin motion of the electrons. The orbital motion of the electron are tied into the nuclear configuration. Hence magnetic moment due to spin motion of the electron is considered.

$$\mu_m = 2\sqrt{s(s+1)}\ B.H. \quad \text{——} ①$$

Where is the spin quantum number. for a molecule or ion containing a number of unpaired electrons.

$$\mu_m = 2\sqrt{S(S+1)} \quad \text{——} ②$$

for are unpaired electrons $S = 1/2$
for n unpaired electrons $S = n/2$
equation ② becomes.

$$\mu_m = 2\sqrt{\tfrac{n}{2}\left(\tfrac{n}{2}+1\right)}$$

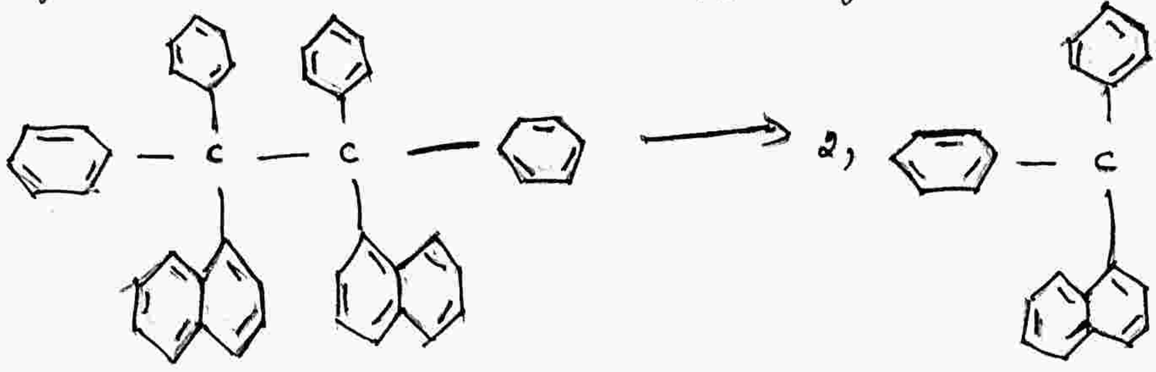
$$\mu_m = \sqrt{n(n+2)}$$

By knowing the number of unpaired electrons (n) the magnetic moment (μ_m) can be calculated. The number of unpaired electron may be calculated if we know magnetic moment.

2.17 Application of magnetic susceptibility measurements:-

i) Study of free radical:-

free radicals are paramagnetic. magnetic susceptibility measurements give an idea about the extent of dissociation of a compound into free radicals. molar paramagnetic susceptibility of α-napthyl diphenyl methyl dissolved in benzene was found to be 140×10^{-6} the corresponding value for one electron is 1300×10^{-6}. This shows that only a fraction of the original substance is in the free radical form.



α - napthyl diphenthyl methyl radical

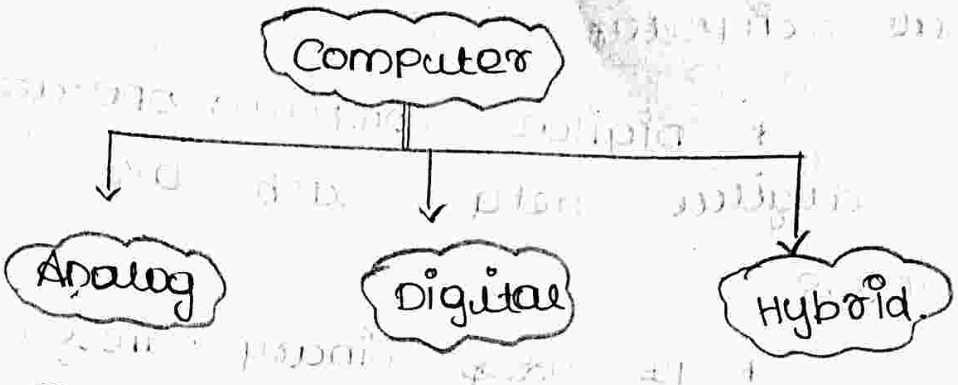
$$\text{Percentage dissociation} = \frac{140 \times 10^{-6} \times 100}{1300 \times 10^{-6}}$$

$$= \cdot 11\%.$$

ii) Application to ions:-

most of the ions of transition and inner transition elements are paramagnetic. The spin only magnetic moments of same.

TYPES Of computer.



Analog computer

* Analog computer is a computing device that work or continow ronge of valuet

* Analog computer gives approximate result sine they deal with quantities that very continauly.

* Generally deals with physical varioble such as
* voltage
* pressure.

* temperature.

* speed etc.

Digital computer

* Digital computer operates on digital data such are numbers.

* It uses binary number system in which they are only digit 0 and 1

* Each one is called a bit

* they are two levels are known as logic 0 and logic 1

* Digital computer can give the result with more accury and faster rate.

Hybrid computer

* A hybrid computer system is a combination of

of desirable featureal of analog and digital computer.

* It is mostly used for automatic operation of complicated phycal processes and machines.

Different components of computer.

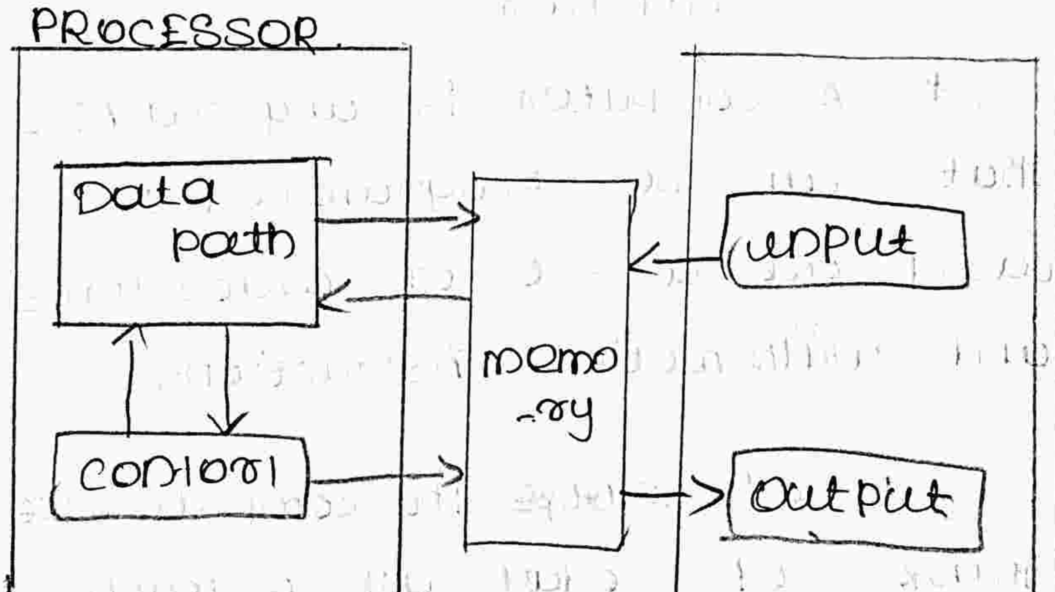
Computer.

* A computer is any machine that can be programmed to carry out a set of algorithms and arithmetic instructions.

* Of course the computer we think of today all so much more that - and I'm talking beyond just being machines used to play games and watch videos of chat on the internet!

componets of a computer.

* the five classic components of a computer are briefly decribed below Each components is discussed in more detail in its own section the operation of the processor is best under shood in terms those componets.



Computer components

Data path

* manipulates the data coming through the processor. It also provides a small amount of temporary data storage.

control

* generates control signals that direct the operation of memory and the data path.

memory

* holds, instructions and most of the data for currently executing programms.

input

* external devies such as key boards mice disks and networks that provide input to the processor.

out put

* external devices such as displays, printers, disks and networks that data from processor.

variables

* variables a symbolic name associated with a value and whose associated value may be changed.

* In programming a varibul is a container to hold data.

* To indicated the storage each variable shoud be given a unique varible names are just the symbotic representation of a memory location.

For Example:

* int player sore = 95

Here player score is a variable of int type here the varible is assigned an integar value95

Bits and Bytes

Bit

* the bit is a basic unit of information in computing.

and digcal commanioction. the name us a postmantiaw of binary digit the bit represents a logical state with one of two posible values those values are most commonty as "1" or "0" but other represented such as true/false yes/No, +/- on/of are common.

Byte

* the byte is a unit of digctal information that most commonly of eight bits Histascalty the byte was the number of biter used to encate a single charactor of teat in a computer and for this reason it is the smallest addressable unit of memory in many computer To disambiguate arbitrarity sized byter from the common 8-bit definition network such as the Internet protocol refer an 8 bit byte as an oter (8)

Binary number system.

* A Binary number system is one of the 4 types of number system in computer applications where binary numbers are represented. by only two symbols digits the binary numbers here are expressed in the base 2 numeral system for example is a binary number Each digit in this system is said to be bit.

there are 4 different types of the number system.

- * Binary number system(base 2)
- * Octal number system (base 8)
- * Decimal number system (base 10)
- * Hexadecimal number system (base 16)

Binary Number system :-

* According to digital electronics of mathematics a binary number is defined as a number that is expressed in the Binary system base 2 numeral system. It describes numeric values by two separated symbols 1(one) or 0(zore) the base-2 system is the positional notation with 2 as Radix

* It is used in all latest computers and computer based devices because of this direct implementation in electronic ciricitus using logic gates Every digit is refered as "Bit"

Bit :-

* A single Binary digit is Bit A binary number consists of several bits

Examples :

* 1010 is a 4-bit binary number

* 1000001 is a 7-bit binary number.

Radix:-

* Binary system operates in digit 0-1 represents number & the Base is known as Radix

Binary number Table:-

Some of the binary notations of lists of decimal number from 1 to 30 are mentioned in the below list.

Number	Binary number	Number	Binary Number	Number	Binary Number
1	1	11	1011	21	10101
2	10	12	1100	22	10110
3	11	13	1101	23	10111
4	100	14	1110	24	11000
5	101	15	1111	25	11001
6	110	16	10000	26	11010
7	111	17	10001	27	11011
8	1000	18	10010	28	11100
9	1001	19	10011	29	11101
10	1010	20	10100	30	11110.

for eg:- 1235

thousand.	Hundereds	times	ones.
1	2	3	5

the above table can be described as.

thousand	Hundereds	Tens	ones.
10^3	10^2	10^1	10^0
1	2	3	5

[any value to the exponent zero is one]

$$1235 = 1\times10^3 + 2\times10^2 + 3\times10^1 + 5\times10^0$$

this can also be shown in the following manner.

	thousands	Hundreds	ones	Tens.
Decimal	10^3	10^2	10^0	10^1
Binary	2^3	2^2	2^0	2^1

$$1235 = 1\times2^2 + 2\times2^3 + 3\times2^1 + 5\times2^0.$$

Position in Binary number system :-

* In the Binary system, we have ones twos fours, etc...

for eg :- 1011.110.

It is shown little this.

$1\times8+0\times4+1\times2+1\times\frac{1}{2}+1\times\frac{1}{4}+0+\frac{1}{5}$

$= 11.75$ in Decimal

As we move more left the number place gets bigger

the first digit on the right is always values 1/2 & as we move more right the In the example given above..

In the example given above.

- * "10" shows "2" in decimal
- * "1" shows half
- * So "10.1 in binary is 2.5' in dismal.

Binary Arithemetic operations.

* we can perform addition subtraction multiplication division operations on Binary number.

Binary Addition

* Adding two binary number with give a binary number itself

binary number is given in the table below

Binary	number	Addition.
0	0	0
0	1	1
1	0	1
1	1	0

For example

```
  1101
+ 1001
 10110
```

Binary subraction

* subration of two single binary number is given below.

Binary number		subraction
0	0	0
0	1	1
1	0	1
1	1	0

For example.

```
   1101
(-) 1010
   0111
```

multiply 1101_2 & 1010_2

```
   1101
   1010
   ----
   0000
   1101
  000
 1101
 --------
 10000010
 --------
```

uses :-

* Binary number are commonly used in computer appliations. All the cating languages in computer such as C, C+1 use binary digits 0 & 1 to write a program (or) any digital data, the computer understands only the coded languge therefore these 2- digit number system is used to a set of data (or) information in discreted bits of information.

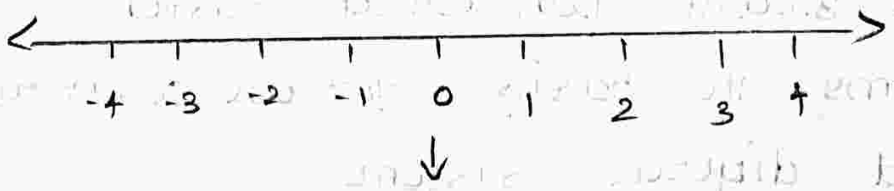
REPRESATATION OF INTEGERS

* Intergers are whole number or fixed point number with radix point fixed after the least significant bit

* Intergers are whole number with a range of values supported by a particular machine

* computer use fixed number of bits to represent an Integer.

Integers number line



zero is neither positive nor negative.

* Generally integers occupy one word of Storge and sine the word sizes of machines very (typically for 32 bites), the sizes of an integer that can be stored depends on computer.

* c has three classes of integer stroage namely short int long int in both singed and forms.

INTEGERS TYPES

short int
int
long int

Conversion of binary to decimal:

* Binary numbering system forms the basis for all computer and digital system

* the decimal or denary counting system uses the Base-of-10 numbering system where each digit in a number takes on one of passible a values called digits from 0 to 9

Eg: 213 (Two Hundred and thiteen)

* But as well as having 10 digits, the decimal numbering system also have the operations of addition (+) subtraction (-) multiplication (x) and division (÷)

* In a decimal system each digit has a value ten times greater than is previous number and this decimal numbering system uses a set of symbol, b, together with a base, q, to determine the weight of each digit with in a number.

$$N = b_n q^n \ldots b_3 q^3 + b_2 q^2 + b_1 q^1 + b_0 q_0 + b_{-1} q^{-1} + \ldots \text{etc}$$

where

N is a real positive number

b is the digit

q is the base value

and integer i can be positive negative (or) zero.

the Decimal Numbering System

* In the decimal or denary numbering system each integer number column has values of units, tens, hundreds, thousands etc as we move along the number from right to left, then each position to the left of the decimal point indicates an increased positive power of 10 and a base of 10 or modulo - 10 with position of each digit in the decimal system indicating the magnitude or weight of the digit as a is equal to 10 (0 through 9) the value of any decimal number will be equal to the sum of its digits multiplied by their repective weights

the Binary numbering system.

* It follow the Same set of rules as the decimal numbering system, But unlike the decimal

system which uses powers of ten the binary numbering system works on powers of two giving a binary to decimal conversion.

Binary digit

MSB LSB

2^8	2^7	2^6	2^5	2^4	2^3	2^2	2^1	2^0
256	128	64	32	16	8	4	2	1

1 0 1 1 0 0 1 0 1

Binary values.

* By adding together All the decimal number values from right to left at the positions that are represented by a "1" gives us (256)+64+32+4+1=367

Repeated Division by 2 (method)

* Dividing each decimal number by '2' as shown will given a result plus a remainder

system which uses powers of ten the binary numbering system works on powers of two giving a binary to decimal conversion.

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2^8	2^7	2^6	2^5	2^4	2^3	2^2	2^1	2^0
256	128	64	32	16	8	4	2	1
1	0	1	1	0	0	1	0	1

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Repeated Division by 2 (method)

* Dividing each decimal number by '2' as shown will given a result plus a remainder

* If the decimal number being divided is even then the result will be whole and the remainder will be equal to "0"

* If the decimal number is add then the result will not divide completly and the remainder will be a "1"

Number of Binary Digits (bits)	Common Name.
1	Bit
4	Nibble
8	Byte
16	word
32	Double word
64	Quad word.

Number of Bytes	common Names
1,0,24 (2^{10})	kilobyte (kb)
1,048,576 (2^{20})	megabyte (mb)
1,073,741,824,(2^{30})	Gigabyte (Gb)
a very long number (2^{40})	Terabyte (Tb)

* A BIT is the abbreviated terms derived from Binary digit

* A Binary system has only two states Logic "0" and Logic "1" giving a base of 2.

* A Decimal system was different digits 0 to 9 giving it a base of 10

Number system and mutual conversion

number system

* computer architecture supports following number system.

* Binary number system
* octal number system
* Decimal number system
* Hexa decimal number system.

Binary number system

* A Binary number system has only two digits 0 and 1 the base of binary number system 2

Binary denotes binary prefix

Example : $(10101)_2 = 10101\,B$

$= 1\times 2^4 + 0\times 2^3 + 1\times 2^2 + 0\times 2^1 + 1\times 2^0$

$= 1\times 16 + 1\times 4 + 1\times 1$

$= 16 + 4 + 1 = 21$

$(1010)_2 = 2\times 1 \quad (21)_{10}$

Octal number system

* octal number system has only (8) digits 0 to 7 0,1,2,3,4,5,6, 7. number system the base to octal number is 8.

Example:

$(27)_8 = 2\times 8^1 + 7\times 8^0$

$= 2\times 8 + 7\times 1 = 16\times 7 = (23)_{10}$

Decimal number

* Decimal number system has only (10) digit 0 to 9 0,1,2,3,4,5,6,7,8,9, the base of decimal number system is 10

Example :

$$(2538)_{10} = 2\times10^3 + 5\times10^2 + 3\times10^1 + 8\times10^0$$

$$= (2\times1000) + (5\times100) + 3(100) + (8\times100)$$

$$= 2000 + 500 + 30 + 8$$

$$= 2538.$$

Hexa Decimal number system.

* A Hexa Decimal number system has (16) phanumeric value 0 to 9 A to F Every number with 0,1,2,3,4,5,6,7,8,9,A,B,C,D,E,F, the base of number system A-10 B-11 C-12, D-13, E-14, F-15,

MUTUAL CONVERSION

* According to martic Luther's writing smalcated Articles: mutual conversation and consolation of Brother and sister is from the gaspel along side.

* mutal conversation and.

consolation connected with confession and forgiveness and finds its particular focus in formals where christains convey to each other world of forgiveness.

* Awarences to the claing

* God's love in claiming us even admidst our sin:

* forgiveness of sins

* Bringing faith

* when we experience such qualities and effects in conversation then we might conclude that such is an occatsion of mutual conversation and consolation.

Introduction to computer.

programming

* A program is a list of instructions that is executed by a computer to accomplish a particular task.

* creating these instructions is programming

* Developing a program is a circular process.

* Analyze the broblem.

* Design a program to solve the broplem.

* code the program

* Test the program

Types of computer / programming Language

* machine Language

* symbolic Langage.

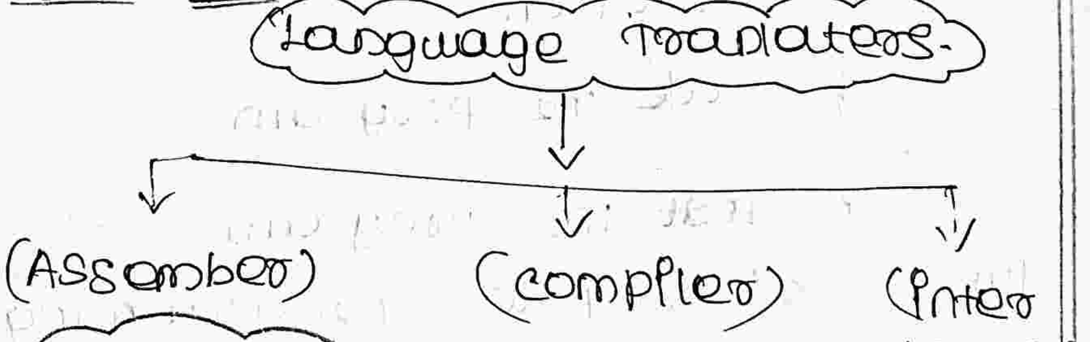
1. <u>New level Languge</u>.

=> New level language is near to machine language Pssembly Language are example of Law level Language.

2) <u>High level Language</u>.

=> High level Language. is near to human language. that language. mostly English word c, c++, Java, cobol, PHb; Basic, and have many other. Language.

<u>Type of Transtation</u>



1. Assembler

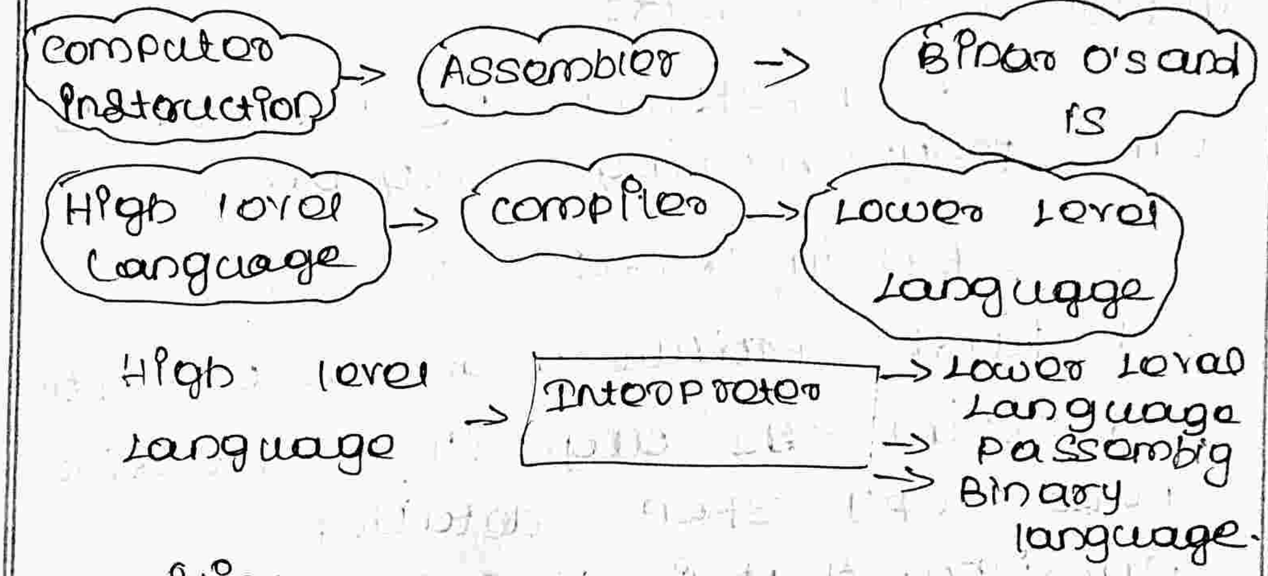
* an assembler translate assemty Lanage into machine code.

2) compiler

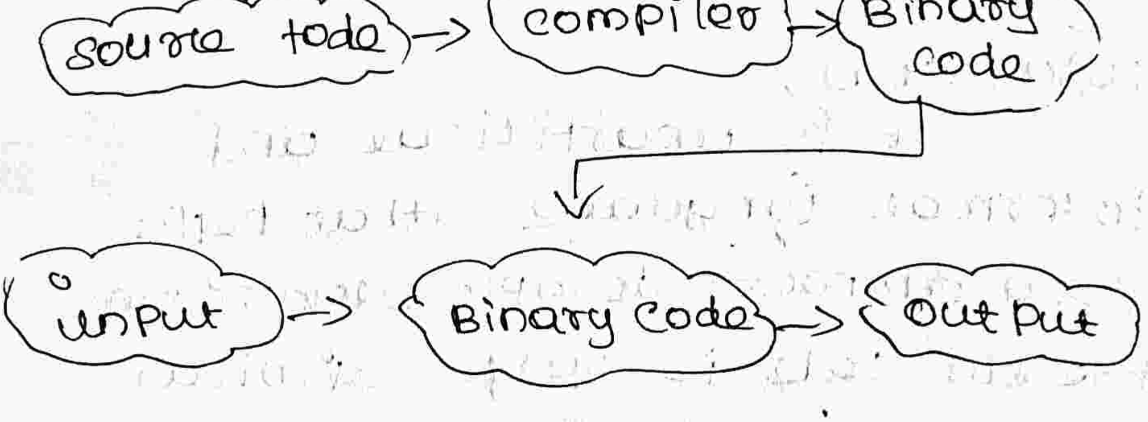
* A computer program that tranlaters an enter set of instructions written in a higher level symbolic Language into machine Language

3) Interpreter

* computer language processor that translator program line by statement by statement



compiling



ALGORITHMS OF FLOWCHARTS

* A typical programming Task canbe devided into two phases.

problem solving phase.

* produe an ordered sequence of steps that describe, solution of broplem.

implementation phase

* impotement the program is same programming language.

STEPS IN PROBLEM SOLING

* First produce a genral algorithm

* Refine the algorithm sucessive woget stepy step detailed algorithm that is very to a computer language.

pesudocode

* is anartificial and informal language that helps programmers deveplo algorithms pseudo code is very similar to everyday English.

EXPRESSIONS , HIERARCHY OF OPERATIONS INBUILT FUNTIONS

EXPRESSION

In computer science , an expression is a syntactic entity in a programming language that may be evaluated to determine its value it is a combination of one or more constands variables , functions and opeartors that the programming language interpretes and computes to produce another value , this process , for mathematical expressions is called evaluation

Expression is often contrasted with statement -a syntactic entity which has no value (an instruction)

Examples

* for examples , $\boxed{2+3}$ is both an arithmetic and programming expression which evaluates to $\boxed{5}$ A

varble is an expression because it denots a value in memore so $\boxed{y+6}$ is also an expression , An example of a relational expression is $\boxed{4 \neq 4}$ which evaluates to false .

VOID AS A RESULT TYPE

* In C and most C-derived languages a call to a function with a void return type is a valid expression, of type void. values of type void cannot be used so the value of such an thrown away.

SIDE EFFECTS AND ELIMINATION:-

* In many programming languages a function and hence an expression containing a function may have side effects An expression with side effect does not normally have the property of referential transparency . In many languages expressions may be ended with a semicolon to turn the expression

this asks the implementation to evaluate the expression for its side-effects only and to disregard, the result of the expression statement that produces side effects "y = x+1;" or fun 1 func 2();"

CAVEATS:

* Notes that the formal notion of a side effect is a change to the abstract stage of the running program.

HIERARCHY OF OPERATIONS:

* In a programming language when an expression involves multiple operations the hierarchy of operations instructs the compilers and inter preters on the order in which the expression consists of operations like addition subtraction multiplication, division exponents and parentheses.

the hierarchy of operations is as follows

* parentheses ()
* Exponents
* multiply or Divide.
* Addition or subtraction.

parenthese

* Execution of the expressions inside the parenthese starting from the innermost parenthese, other parenthese the special characters like brackets [] braces {} and square roots also fall under this category

Exponents

* After solving the operations in the parentheses starting choose the exponants for execution.

multiplication or Division

* the order of multiplication and division in an expression has the third priority perform the multiplication or division operation in the left to right order.

Addition or subtraction

* the order of addition or subtraction in an expression has the last priority perform the addition or subtraction operation in the left to right order.

Example

solve the following expression

$a = 3*2/2+2+6-1+5/8$

$a = 3*2/2+2/2+6-1+5/8$

$a = 6/2+2/2+6-1+5/8$ operation :*

$a = 3+2/2+6-1+5/8$ operation :/

$a = 3+1+6-1+5/8$ operation :/

$a = 3+1+6-1+0$ operation :/

$a = 4+6-1+0$ operation :+

$a = 10-1+0$ operation :+

$a = 9+0$ operation :-

$a = 9$ operation :-

INBUILT functions

*. the processing we have done so far involves matching existing data against a template, and where a match occurs. generating more inferred data, this is much like which you do with a data base using sql and just as with sql in practice you need to be able to combine it with

and so no

* Built in functions are properties for which cwm can calculate the object given the subject

* Built in inverse functions are properties for which cwm can the subject given the object

* A complete list of builtin function is available

side of a rule

* there built a function given alow you to use basic properties of strings and number in your rules they also allow you to do pragmatic things such as pick up command line paranetes and variables, which allow the whole rules system to be parame terized they also allow you do do something else they allow you to make rules which interegate the web parse documents and took at the contents of documents.

Elements of Basic Language.

1) character set

* A BASIC language, as any other langauge has its own alphabet of character set. All the quantities defined and used in BASIC are construced by using the character set.

letter -> A, B, C ---- Z

a, b, c --- z

Digits -> 0, 1, 2, ----- 9

special character -> +-*/(),, $<>;

Blanks -> In the text we shall denote a blank by the character ^

Eg. 30 PRINT "GOVIND" ; "^", "SINGH"

outer -> (single outer) or (Double outer)

[i -> different quantites appearing in the list of the PRINT statement can be saparated by semicolons)

2) constants and variables.

constants

* the quantities whose value camot be changed is a program are referred to as constants

1) Numexic contants

2) Non - numexic of litteral of string constants.

a) Numeric constants

* A constant of the number 0, 1, 2 - - - 9 there

* Integer constant

* Real constant

1) Integer constant

* A number with out on explicit decimal is called integer constant (i.e whall number) Eg, 1x20, 300

2) Real constant :

* the number includer a decimal point Eg // 22 . 33

33 is called it's practional perstand 22 is it integer past

Example

/* variable to store long value*
-long a;

/* variable to store folat value *, float b;

BASIC KEYWORDS AND COMMANDS

key words

* key work are the words where meaning has been explained to c compiler.

* they have a specific meaning and they implement specific c languge feature

* In terms of SEO they are the words are pharases that searcher enter into search engines also called search queries.

COMMANDS

* key work cannot used as variable or constant names

* key words are written in lowercase letter

* key words are reserved words which ax propose.

Ex there ax 32 key words in c are given below.

auto	double	int	struct
break	else	long	switch
case	enum	register	typedef
char	extern	return	union
const	float	short	unsigned
do	if	static	while

7EW EX :

1) auto

* the auto keybored declaroo teo example

auto int var1 :

2) char

the char key words declares a variable 7oo example.

char alphabet ;

LOUICAL OPERATOR and RELATIVE OPERATORS

LOUICAL OPERATORS

* A logcial opearator is a symbol or word used to connect two or mere expressions such that the value on tho of the original Expression and on the meaning of the operater common logkal opeators AND , OR, and NOT

DISCUSSION :

* with in moast language a expression that valed Booleon data type value are dipvied into two group on group and the other group user logcal opeaators with in this expression .

In most languages there are strict rules for forming proper logical

6>4 $$ 2<=14

6>4 and 2<=14

Logical operator

* An operator used to create complex Boolean expression.

truth tables.

* A common was to show logical relationship.

Examples

25<7||15 >36

15 >38||3<7

14 > 7&&5<=5

Discussion

* the relational operators are often used to create a tea expression that controls program flow operator symbol and lor names can very with different programing languages most program language use relational operators to the following

operators	meaning
<	less than
>	greater than
<=	less than or equal to
>=	greater than or equalto
==	equality (equalto)
!= or <>	equality (not equal to)

Examples

9 < 25
9 > 14
9 <= 17
9 >= 25
9 == 13

9! =13
9<>25

RELATIONAL OPERATOR:

* An operator that gives a boolean value by evaquation the relationship between two operands

COMPILED LANGUAGE

* A compiled Language is a porgramming when imprment ax typically compiler and not interpreter.

INTERPRETED LAGUAGE

* An interprect language is a type of programming language for.

implementations exeue instructions dencetly and freally with out prevously comping a program into machine - lananage instructions.

COMPILED LANGUAGE VERSUS INTERPRETED LANGUAGE

COMPILED LANGUAGE	INTERPRETED LANGUAGE
* the code to compiled language can be excuted directly be the computer CPU	A program written in a interpreted language is not compiled it is interporeted.
the soure code must be trans formed into machine redable instructions prior to execution	It does not compile the soure code into machine language prior to runing one program.

DEBUGGING

DEBUGGING

* Debugging is the process to detecting and rcroving to existing and potential errors also called as bugs in a software cake that can cause it to behave unexpectedly (or) crash To prevent.

operation of a software (or) sytem debugging is used to find and resolve bhgs (or) defects.

BASIC STEPS IN DEBUGGING ARE

- Recognize that abong exist
- Isolate the source of one bug
- Identity the cause of the bug
- Determine a fix for one bug
- Apply the fix and test it

simple programs using these concepts for

Calculating the rate constants

* In this example you will learn to create a simple calculator in c programming using the swich statement

* To understant is example you should have the knowledge of following c programing topics.

- c swith statements
- c break and continue.

simple calcultor (using swich statement)

```
# include <stdio.h>
int main () {
    char operator ;
```

```
        double  first second:
         printy  ("Entor an operator (+,-, *):");
        Scanf  ("%C" . α operator):
        printy (" Enter two operands: ")
       Scanf ("% lf "; first ; and second):
swich  (operator)}
 case'+' :
        printly (" %.lf f + %. . . . . " % = %. . " + ")
first  , second , first + second , ; break;
case :-
   printly (%. ," f - %. . . " f  = %. " f", first
second ,, first - second ) : break ;
case'* . ;
   printly (" %. . . " f * %. " f = %. ",f ", first,
second , first * second ) : break:

   printly (" Enter! operator is not corect") :
  }
   return 0 :
  }
Output :
   Enter  an  operator (+, -, *,) : *
   enter two operator  : 1.5
   45
```

1.5 * 4.5 = 6.3

the * operator entered by the user is stored in operator and the two operands 1.5 and 4.5 are stored in first and second respectively.

Normality of a Solution

What is Normality

* Normality in chemistry in of the the expression used to define the concentration of a solution. Referred it is mainly used us a measure of reactive species in a sand during titration reactions involving and base chemistry.

Normality formula:

* N = molarity ~~x~~ molar mass x [Equivalent + mass]

* molarity x Basicity = molarity x Acidity Normality is of often denoted by the letter N. Some of the other units of normality are all expressed

calculation of Normality in titration

* Titration is the process of

gradual addition of a solution of a known concentration and volume with another of unknown concentration until the reaction approaches its neutralization to find the normative of the acid and base titration.

$$N_1 V_1 = N_2 V_2$$

N_1 = Normality of the Acidic solution

V_1 = volume of the solution.

$V_R = (N_a m_a v_a + n_b m_b v_b + b_c m_c v_c + n_d m_d v_d + v_a + v_b + v_c + v_2)^{-1}$

matrix addition:

* A matrix addition takes two input matrices B and C produces one output matrix A. Each element of the output matrix A is the sum of the corresponding

ie) $A[i][j] = B[i][j] + C[i][j]$

matrix addition rules:

* matric A and matrix B

$$A = \begin{pmatrix} 1 & 2 & 3 \\ 7 & 3 & 9 \end{pmatrix} \qquad B = \begin{pmatrix} 5 & 6 & 7 \\ 3 & 4 & 5 \end{pmatrix}$$

$$A+B = \begin{pmatrix} 1+5 & 2+6 & 3+7 \\ 7+3 & 3+4 & 9+5 \end{pmatrix}$$

gradual addition of a solution of a known concentration and volume with another of unknown concentration untill the reation approaches it neutralization to find the incmative of tho acid and base titration.

$$N_1V_1 = N_2V_2$$

N_1 = Normality of the Acidic solution

v_1 = volume of the solution.

$VR = (N_a m_a v_a + n_b m_b v_b + n_c m_c v_c + n_u m_u v_u + v_a + v_b + v_c + v_2)^{-1}$

matrix addition.

* A matxix addition takes two input matries B and C produces one output matrix A - Each element of the output matrix A is the sum of the coroponding

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$$A+B = \begin{pmatrix} 1+5 & 2+6 & 3+7 \\ 7+3 & 3+4 & 9+5 \end{pmatrix}$$

$$A+B = \begin{pmatrix} 6 & 8 & 10 \\ 10 & 12 & 14 \end{pmatrix}$$

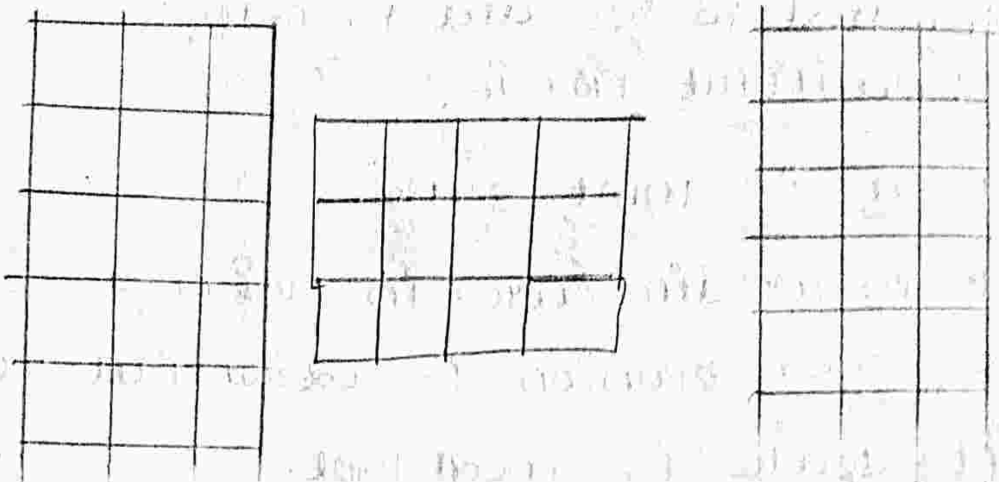
I must emphasize that in order to add two given matrias they should have the same size or otherwise different sizes of dimention is undefined!

Algorithm to perform matrix Addition.

```
Step : 1   Input the matrix 1 elements
Step : 2   Input the matrix 2 elements
Step : 3   Repeat from i=0 to number
           of rows
Step 4 :   Repeat from j=0 to number
           to columns.
Step 5 :   matrix 3 [i] [j] = matrix [i](j)
           + matrix [i) [j]
Step 6 :   print matrix 3
Step 7 :   End.
```

matrix multiplication

* In mathematics particularly in linear algebra matrix multiplication is a binary operation that produces a matrix from two matrices for matrix second matrix



for matrix multiplication the number of colums in the first matrix must be equal to the number of rows is the scecond to the number of rows in the second the result matirx must be has the number to rows of the first and the number to rows to the second matrix

* matrix multipilcation was first described by the french mathematician Jacques philipe marie Binet in 1812 [3] to represent the composition of computing matrix products is a central operation in all comulational applications of lines algebra.

Statrtical analysis defined

* manufactures use statixics to weave quality into beautiful

to bring [illegible] to the and to help make beautiful music.

Pros of a 4 point scale.

* In certain cases in which a specific user opinion is essential the 4 point scale is most ideal.

* Best for recording opinions on services / product which the user has used / experienced.

Cons of a 4 point scale.

* A 4 point likert scale in observed to distort the results

* A 4 point scale forces a choice when a has opinion.

Formulas.

* Population mean $= \mu = (\Sigma x_i)/N$
* Population standard deviation. $= \sigma = \text{sqrt}[\Sigma (x_i = \mu^2)]$
* Population of population proportion $= \sigma_{\hat{p}} = PQ/n$
* Population variance $= \sigma^2 = \Sigma (x_i - \mu^2)/N$
* Standardized score $= z = (x - \mu)/\sigma$

No	category	Applications	varius
1)	web Browser	Internet explorer Fire fox ESR google chrome Adobe Flash player	11 45.70 55.0.222.3.37 24.0.0.194.
2)	Email client	thunderbird Firezilla	45.6.0 3.24.0
3)	communication	wins scp Teraterm ISSI+2 (UTF-2)	5.9.3 4.93
4)	micro soft office	microsoft office professional pluss 2016	world 2016 excel 2016 pwer point 2016 Access 2016 publisher 2016
5)	PDF	Acrobak Reader DC	2015.023. 20053
6	Editor	terapad Sakura Editor	1.09 2.201

7)	multi media	VLC media player	2.27
8)	Graphics	GIMP	2.2.13
9)	Archiver	LHmelt	1.65, 3.6
10)	other	Arcolig maxima	10.4.1 5.39.0.

List of computer soft ware and their uses in chemistry.

* this is a list of saft war to simulate the material and their energy balance to chemical process plants contorl system. check out process simulation dynamic, & operator training turins.

* there are a number of every problems between system contrel and automation which originate from the common principle where by the computer is used to recive or computer is chemistry

is the field of quantum mechanical computation.

* soft wore is a set of inxruction dara or progoams used to operate computers and excute specific takes opsosite of hard wore which describes the physical aspects of a computer soft wore is a gextic term used.

* the but it bluntly soft wore is what makes almost every thing you see possible the derktop the wep broco ser you name it pobaly in the day of ms dor commands and games had to be loades an run of that system would other wise ran on then along came windows.