c/w

Chemical Bonding and shape of Molecules

1. Valence Shell

The outermost shell of an atom is called valence shell.

2. Valence Electron

The number of electrons present in the outermost shell of an atom is called valence electron

3. Octet Theory or Octet Rule

The tendency of an atom of an element to acquire ~~the~~ ~~nearest in~~ electron to nearest inert gas configuration (i.e 8 electron) to their outermost shell is called octet Rule.

Some ~~electron~~ elements bear more or less number of electron than ~~oct~~ octet rule in their molecules which is called exception of octet rule.

For example : 'B' in BCl_3
'P' in PCl_5 etc.

4. Electrovalent Bond

The electrostatic force of attraction which holds cation and anion together is called electrovalent bond or ionic bond.

During the formation of this bond, metallic atom loose its valence electron to form cation and non-metallic atom gains the electron loose by metallic atom to form anion. An electrostatic force of attraction holds this ions together which is called electrovalent or ionic bond. The compound formed due to this bond is called electrovalent or ionic compound.

For example:

Formation of NaCl

i. Sodium atom loose its one valence electron to form cation.

$Na \longrightarrow Na^{+} + e^{-}$

ii. Chlorine atom gains one electron and form anion.

$Cl + e^{-} \longrightarrow Cl^{-} + EA$

iii. An electrostatic force of attraction holds these ions together to form electrovalent or ionic bond

$Na^{+} + Cl^{-} \longrightarrow Na^{+} ::: Cl^{-}$

5. Electrovalency

The number of electron lost or gain by an ~~a~~ ~~an~~ atom during the formation of electrovalent bond is called electrovalency.

Factors affecting formation of ionic compounds

1. No. of valence electron

The atom having 1, 2, or 3 valence electron forms cation and the atom having 5, 6 or 7 valence electron can form anion.

2. Ionization Energy

~~The ma~~ If the magnitude of ionization energy be small, greater will be the formation of cation that will ~~favor~~ favour the formation of ionic compound.

3. Electron affinity

Higher the value of electron affinity, easier will be the formation of anion and also favours the formation of ionic bond or ionic Compound.

4. Lattice Energy

The amount of energy release when one mole of ionic compound is formed from its ions is called lattice energy.

Higher the value of lattice energy of the ionic compound, greater will be the ease of formation of ionic compound.

5. Electronegativity
Higher the value of electronegativity difference between anion and cation, stronger will be ionic bond.

Properties of ionic Compound

1. Physical State
Ionic compounds are formed by strong electrostatic force of attraction between cation and anion so that they exists in solid crystalline form at room temperature.

2. Solubility
Ionic Compound are highly soluble in polar solvent like water, ammonia solution etc. but insoluble in non-polar or organic solvent

3. Hardness
They are hard, rigid and brittle in nature.

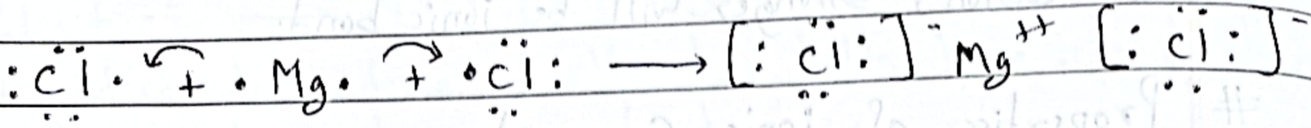
4. Conductivity
Ionic Compound cannot conduct electricity in solid ~~sa~~ state but they ~~&~~ conduct electricity in the molten or aqueous state as they contain mobile ions.

5. Nature of bond
Ionic bond is non-directional in nature due to attraction of oppositely charged ion from all direction.

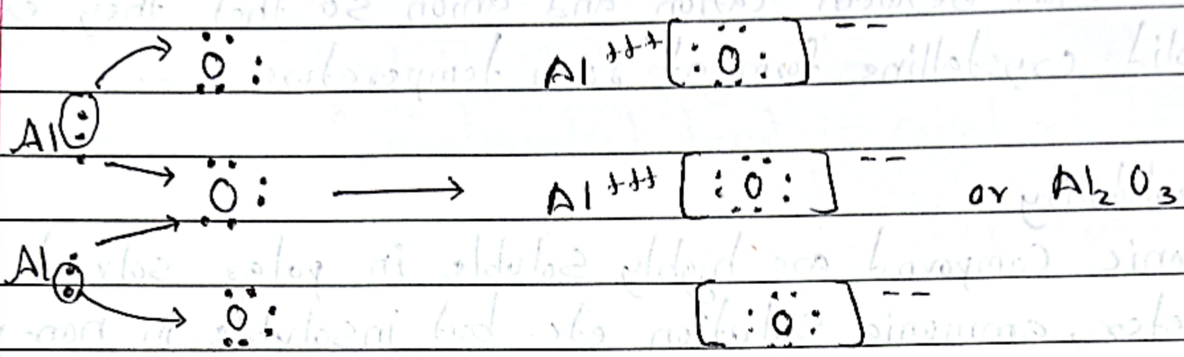
6. Melting and boiling point
Ionic Compound have high melting and boiling point because they require high amount of heat energy to separate ions from crystals.

Lewis Dot formula

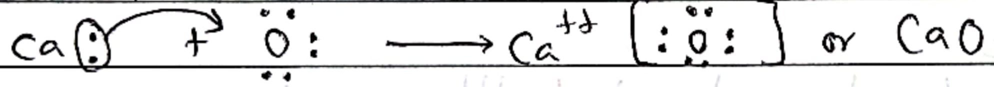
a. Formation of $MgCl_2$



b. Formation of Al_2O_3



c. Formation of CaO

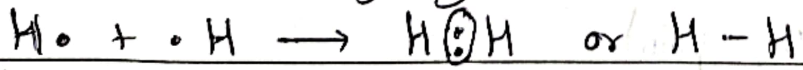


Covalent Bond

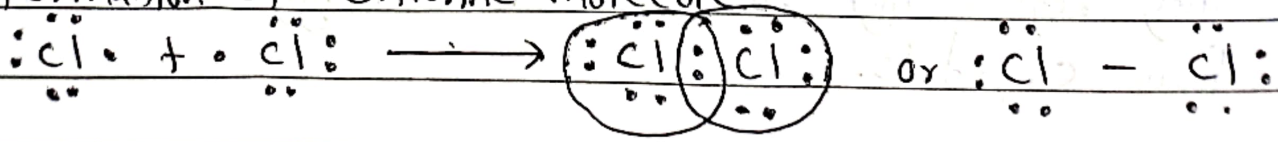
The bond formed by mutual sharing of electrons between combining atoms of the same or different elements is called a covalent bond. It takes place between non-metals. It is represented by a dash (–). The number of electrons that an atom contributes for sharing during covalent bond formation is called ~~covalent~~ covalency. The compounds formed by the covalent bond is called covalent compounds.

Example of covalent bonds:

1. Formation of Hydrogen molecule



2. Formation of chlorine molecule



Properties of covalent Compound

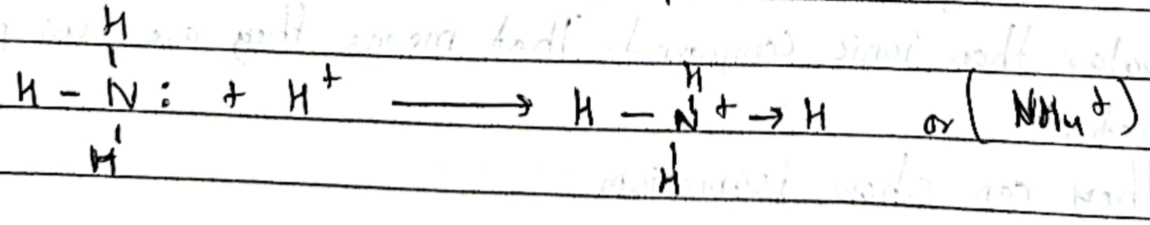
i. Covalent compound exists as gases or liquid and some exist as soft solid.
ii. They are slightly soluble in water but highly soluble in the organic solvent.
iii. Generally, they don't conduct electricity.
iv. They have low melting and boiling points than ionic compound.
v. They are directional in nature.
vi. Covalent compound under molecular reaction which are very slow.
vii. These compound show isomerism.

Coordinate Covalent Bond (Dative Bond)

The bond formed by the sharing of electrons in which the shared pair of electrons is contributed by one of the bonded atoms is called a ~~don~~ coordinate covalent bond. The atom that donates the shared pair of electron is called the ~~donour~~ donor atom and which accepts the shared pair of electrons are called the acceptors atom. This bond is called semi-polar or dative bond. It is represented by an arrow (⟶) pointing from donor atom to acceptor atom.

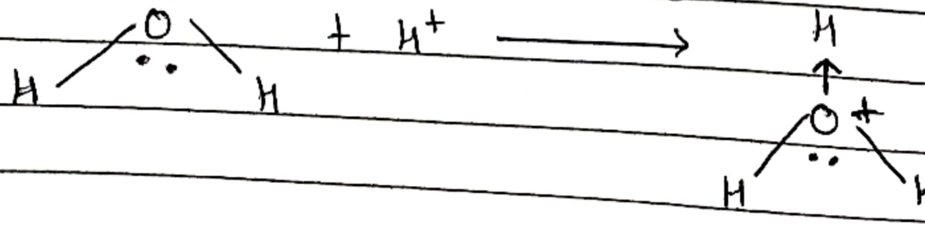
For example:

i. Formation of ammonium ion (NH_4^+).

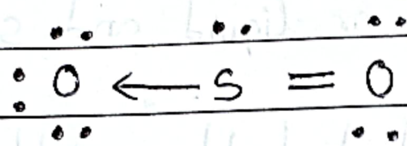


$$H-\overset{H}{\underset{H}{N}}: + H^+ \longrightarrow H-\overset{H}{\underset{H}{N^+}}\rightarrow H \quad \text{or} \ (NH_4^+)$$

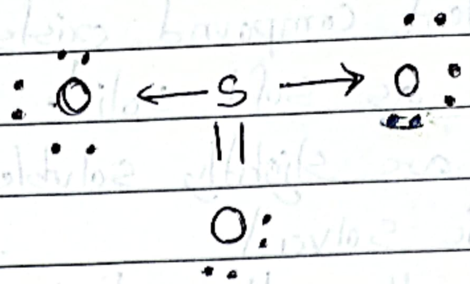
ii. Formation of hydronium ion (H_3O^+)



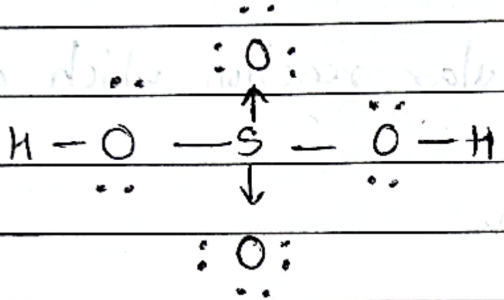
Lewis structure of some coordinate covalent compounds.

i) 

SO_2

ii) 

SO_3

iii. 

H_2SO_4

Characteristics of Coordinate Covalent Bond

i. Coordinate covalent compound are solid, liquid or gas.

ii. Generally, they are insoluble in water but soluble in the organic solvent.

iii. Melting and Boiling points of these compounds are usually higher than covalent compound and lower than ionic compound.

iv. The electrical conductivity of these compound is almost negligible due to non-ionic nature of the compound.

v. These compounds are more polar than covalent compound and less polar than ionic compound. That means, they are semi-polar in nature.

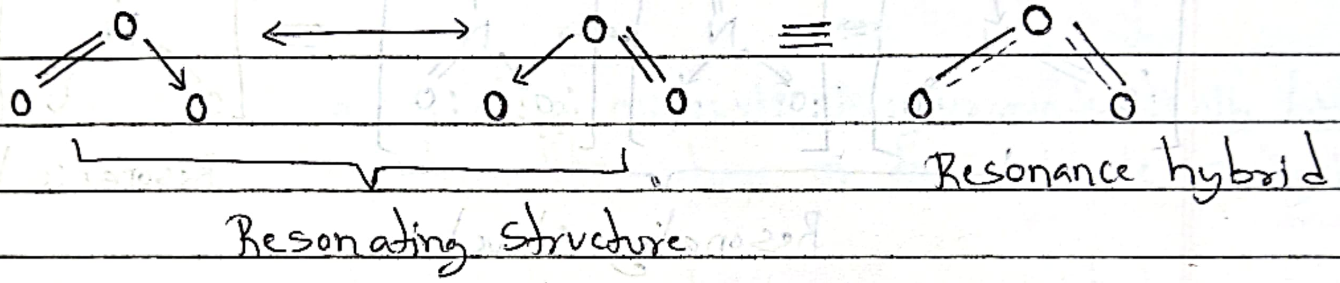
vi. They can show isomerism

Resonance

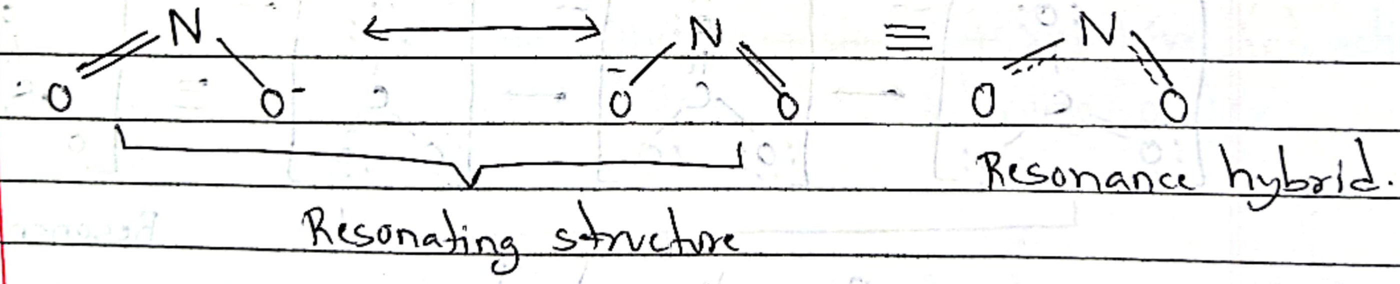
The phenomena in which a molecule or ion cannot be represented by a single structure but represented by more than one structure to explain its properties is called resonance. More than one such structure of the same molecule or ion is called resonating structure. the real structure of the molecule or ion is a hybrid of these structures called a resonance hybrid. It is represented by a double-headed arrow (⟷)

Example:

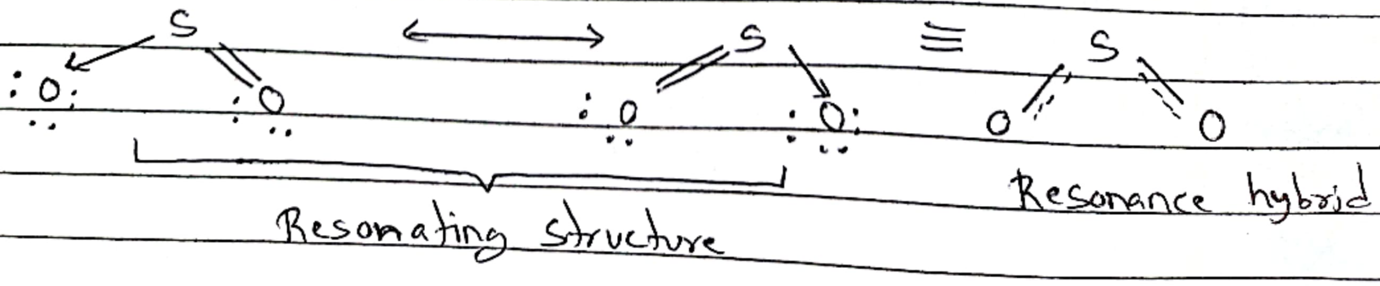
i. Resonance in ozone



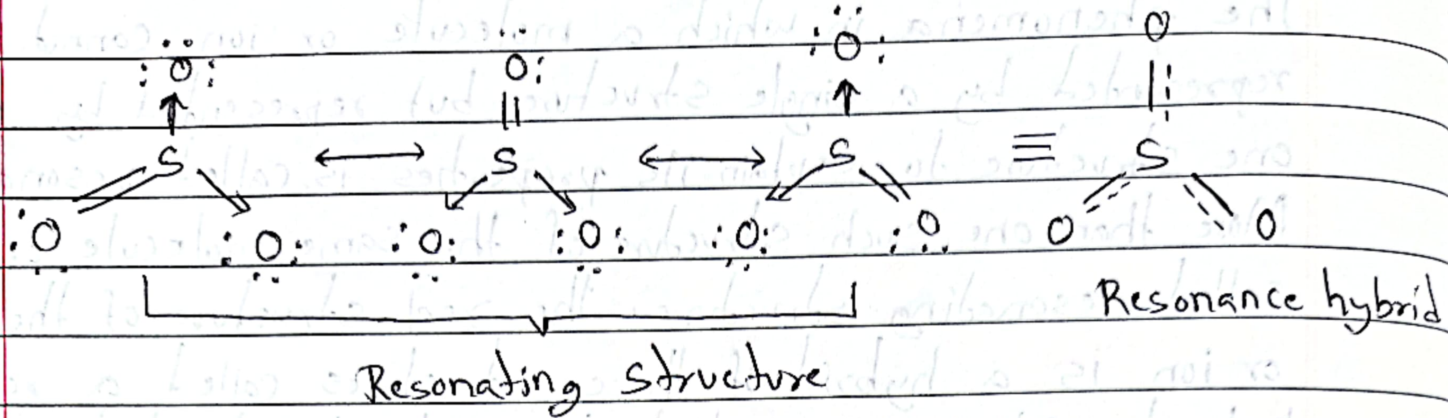
ii. Resonance in NO_2^-



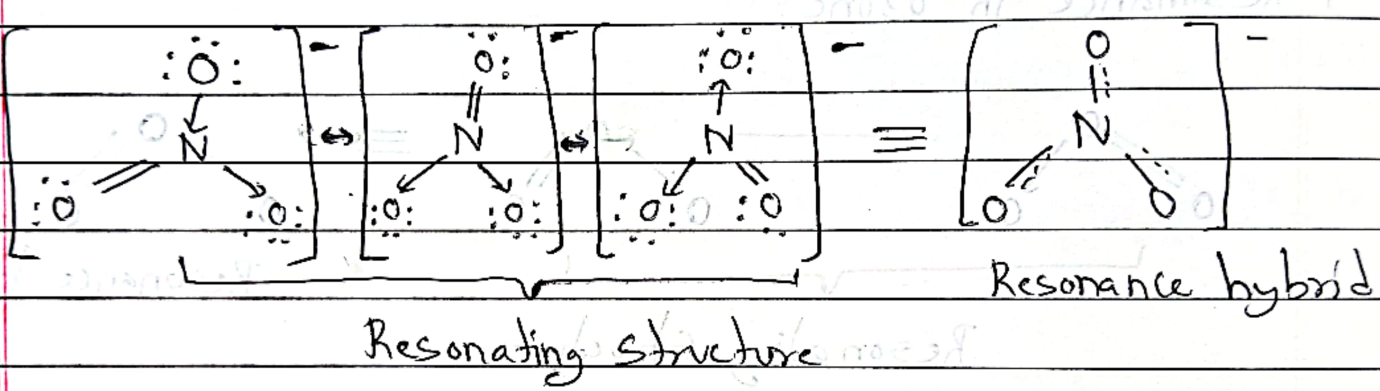
iii. Resonance in SO_2



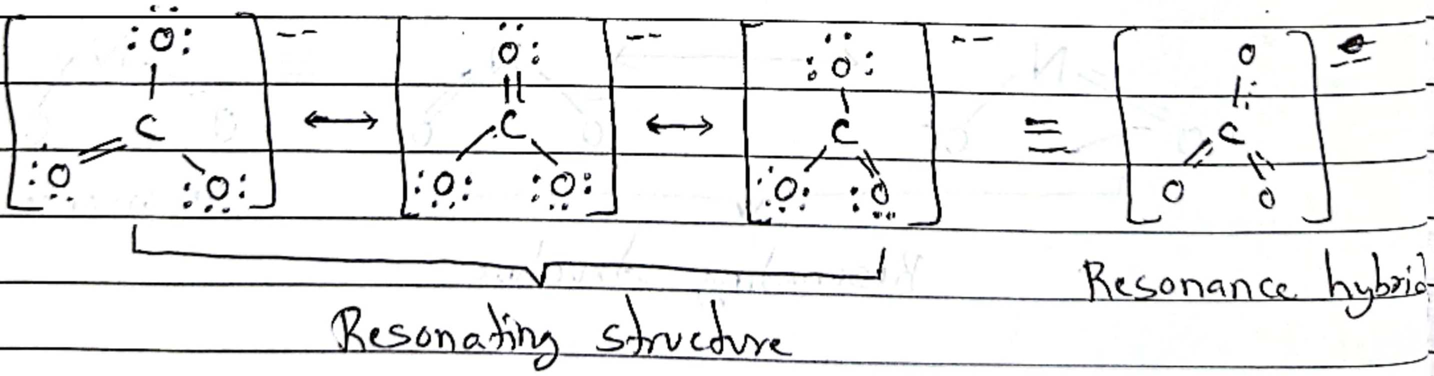
iv. Resonance in SO_3



v. Resonance in ~~SO~~ NO_3



vi. Resonance in ~~a~~ CO_3^{--}



Imp # Valence Shell electron Pair repulsion (VSEPR) theory

To predict the shape of the covalent molecules, Gillespie and Nyholm developed a theory known as valence shell electron pair repulsion theory. The main postulates of this theory are given below:

1. The shape of covalent molecules depends upon the number and nature of electron pair surrounding the central atom. The electron pairs are arranged as far apart as possible so that there is minimum repulsion between them due to which stability is increased.

2. If the central atom of a molecule is surrounded only by a bond pair of electron, the shape of the molecule is regular.

3. If the central atom of the molecule is surrounded by both bond pair and lone pair of electrons, the molecule does not have a regular shape. It is due to the presence of lone pair of electrons. The ~~repulsion int~~ repulsive interaction between the electron pair follows the following order:
lP – lP > lP – bp > bp – bp

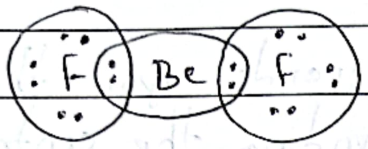
4. The electronegativity of atoms in a molecule also affect the bond angle of the molecule.
i. As the electronegativity of the central atom increases, the bond angle increases.
ii. As the electronegativity of atoms bonded to the central atom increases, the bond angle decreases.

5. This theory considers a multiple bond as a single bond pair of electron.

6. Repulsion between electron pairs in completely filled shell is larger than in incomplete filled shell.

Application of VSEPR Theory

i. BeF_2 Molecule

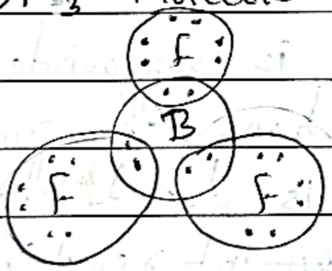


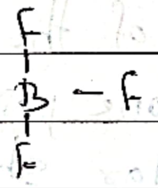
F — Be — F

Linear shape

The central atom Be of the BeF_2 molecule is surrounded by two bond pair of electron. To minimise the repulsion between electron pairs, they must be arranged linearly at 180°. So, the molecule has a linear shape.

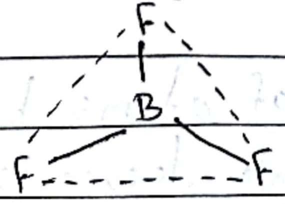
ii. BF_3 molecule





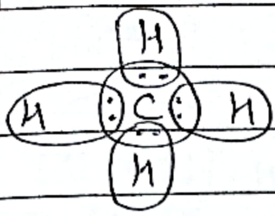
Lewis structure

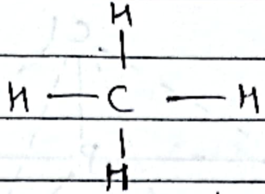
The central atom ~~of~~ B of the BF_3 molecule is surrounded by three bond pair of electron. To minimise the repulsion between electron pairs, they must be directed towards three corners of an equilateral triangle with a bond angle of 120°. So the molecule ~~of~~ has a trigonal planar shape.



Trigonal Planar Shape

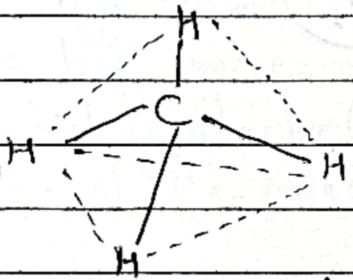
iii. CH_4 molecule





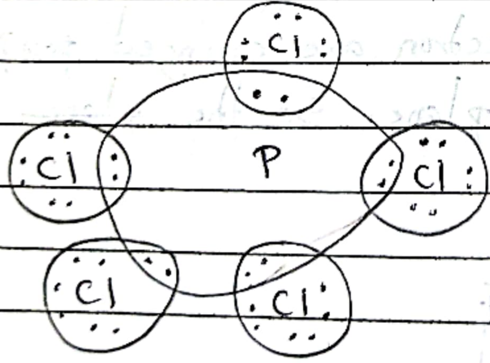
Lewis structure

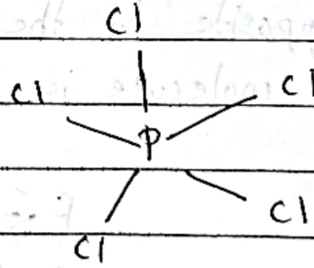
The central atom C of the CH_4 molecule is surrounded by four bond pair of electron. To minimise the repulsion between electron pairs, they must be directed dowards four corners of a regular tetrahedron with a bond angle of 109.5°. So the molecule has a tetrahedral shape.



Tetrahedral shape

iv. PCl_5 molecule

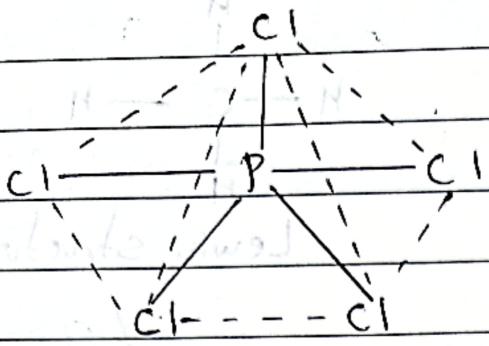




Lewis structure

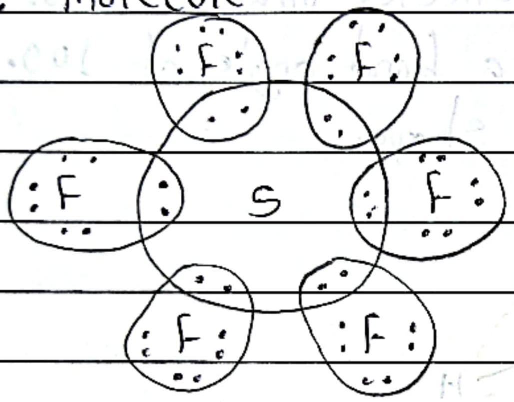
The central atom P of the PCl_5 is surrounded by 5 pair of electron. To minimise the repulsion between the electron pair, three of them lie in an equilateral plane with a 120° angle. The remaining two electron pair are arranged perpendicularly opposite to this plane. So the shape of the molecule is

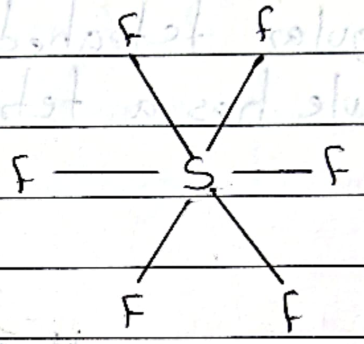
Trigonal bipyramidal



Trigonal Bipyramidal shape

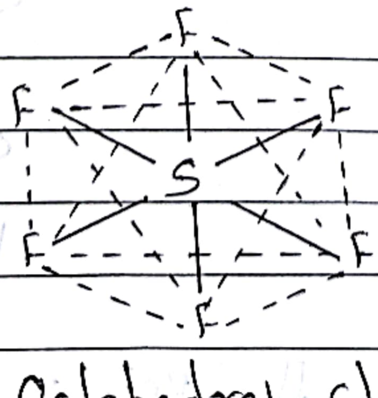
v. SF_6 molecule



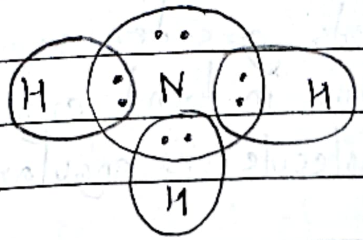


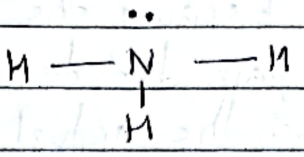
Lewis structure

The central atom of the molecule is surrounded by 6 bond pair of electron. To minimise the repulsion between them, four of them lies in equatrial ~~equodrial~~ plane with an angle of 90°. The remaining two bond pair of electron are arranged perpendicularly and opposite to the equodrial plane. So the ~~plane~~ shape of the molecule is octahedral



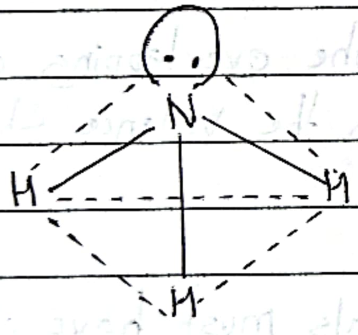
Octahedral shape

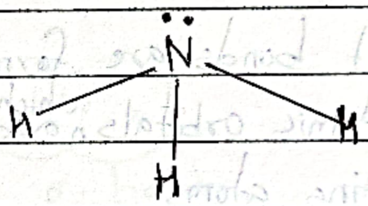




Lewis structure

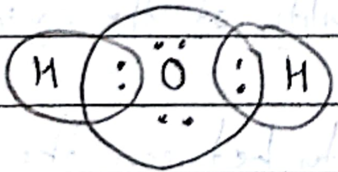
The central atom N of the NH_3 molecule is surrounded by 4 electron pairs. To minimise the repulsion between them, they should be arranged in a tetrahedral manner. So, the expected shape of the molecule is tetrahedral. But, due to the presence of one lone pair of an electron, there is ~~as~~ distortion in the shape because the lone pair exerts greater repulsion to the bond pair due to which contraction in bond angle takes place. So the actual shape of the molecule is pyramidal with an angle of 107.5°

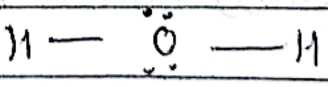




pyramidal Shape

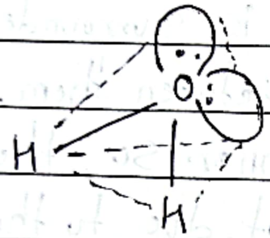
vii. H_2O molecule

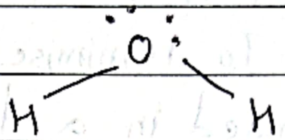




Lewis structure

The central atom O of the H_2O molecule is surrounded by 4 electron pairs. To minimise the repulsion between them, they should be arranged in a tetrahedral manner. So the expected shape of the molecule is tetrahedral. But, due to the presence of two lone pair of electrons, there is distortion in the shape because the lone pair exerts greater repulsion to the bond pair due to which contraction in bond angle takes place. So the actual shape of molecule is angular with an angle of 104.5°.





Bent V-shape (Angular shape)

Valence Bond Theory

To explain the stability of the covalent molecule, a new method to form a covalent bond was proposed by Hitler and London. Following are the postulates of this theory:

1. Covalent bonds are formed due to the overlapping of half-filled atomic orbitals which are presents in the valence shell of participating atoms.

2. For overlapping, the half-filled orbitals must have electrons of opposite spin.

3. After overlapping, the pairing of electrons takes place which decrease energy and increases the stability of the system.

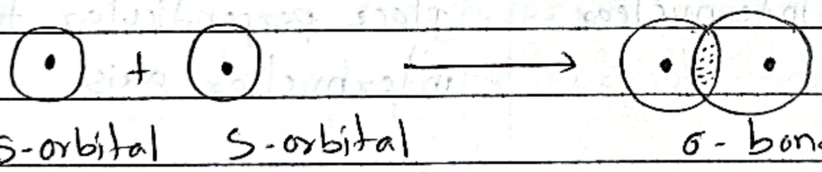
4. Due to overlapping, the electron density between the two nuclei of the bonded atom is increased which causes the formation of a covalent bond.

5. The strength of the covalent bond depends upon the extent of overlapping. Greater the extent of overlapping, stronger is the bond and vice versa.
According to this theory, the covalency of an element is equal to the number of half-filled orbitals present in the valence shell of an atom.

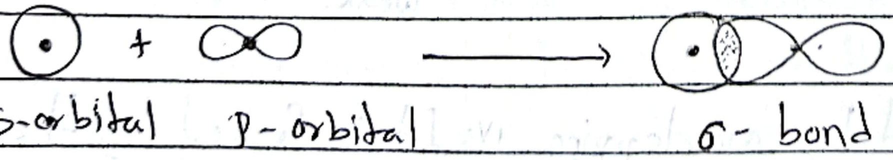
Types of Covalent bond
Depending upon the nature of overlapping, there are two types of covalent bond

1. Sigma (σ) bond:
A covalent bond formed due to head-on overlapping on half-filled atomic orbitals is called a sigma bond. It is ~~due~~ formed due to the following types of overlapping.

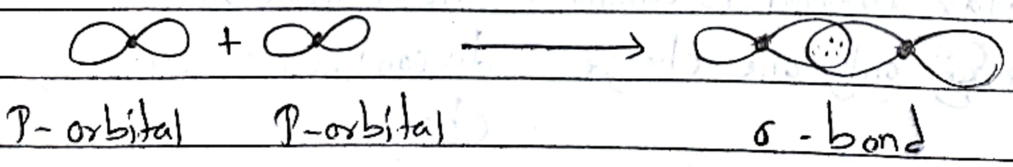
i. S-S overlap



ii. S-P Overlap

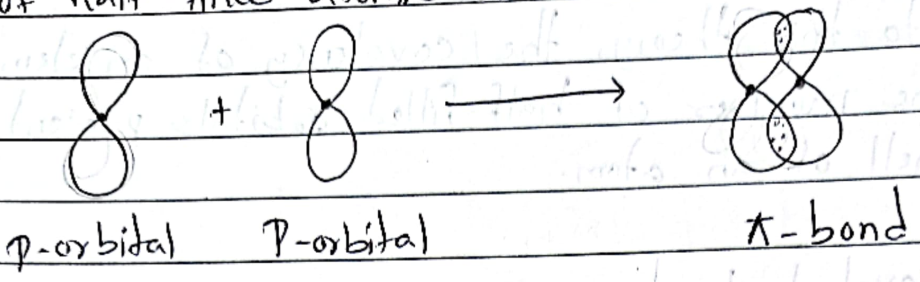


iii. P-P overlap



2. Pi (π) bond

A covalent bond formed due to sidewise (lateral) overlapping of half-filled atomic orbitals is called Pi bond.



Difference between Sigma (σ) and Pi (π) bonds.

σ - bond	π - bond
i. It is formed by end to end, head-on or axial overlapping of half-filled orbitals.	i. It is formed by sidewise or lateral overlapping of half filled orbitals.
ii. Overlapping of orbitals takes place along the internuclear axis.	ii. Overlapping of orbitals takes place perpendicular to the internuclear axis.
iii. The extend of overlapping is large. So the bond formed is strong.	iii. The extent of overlapping is small. So the bond formed is weak.
iv. It is formed by overlapping of s-s, s-p or p-p orbitals.	iv. It is formed by the overlapping of p-p orbitals.
v. The molecular orbital is continuous containing only one charge cloud.	v. The molecular orbital is discontinuous containing two charge cloud.
vi. It can exist alone.	vi. It doesn't exist alone.

vii.	There is a free rotation of atoms around the sigma bond.	vii	There is no free rotation of atoms around the pi bond.

Hybridization

~~It is~~ The process of intermixing two or more orbitals of an atom having comparable energy to give new set of orbitals equal in number to the mixing orbitals having similar shape and same energy is called hybridization.

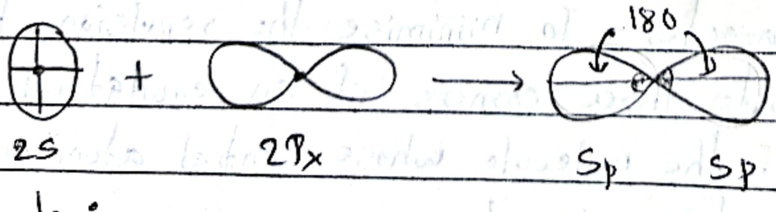
There are mainly 3 types of hybridization.

i. SP - hybridization
ii. sp^2 - hybridization
iii. sp^3 - hybridization

i. SP - hydridization

The phenomenon of intermixing one s-orbital and one P-orbital with comparable energy of an atom to give two hybrid orbitals having an identical shape and the same energy ~~level~~ content is called sp-hybridization.

Each sp hybrid orbital has its 50% s-character and 50% P-character. To minimize the repulsion, they are arranged in a linear manner. So the shape of the molecules whose central atom undergoes sp hybridization is linear.

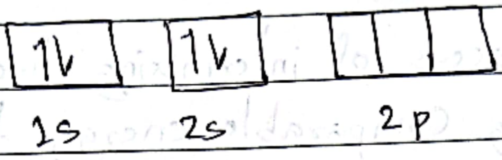


Example:

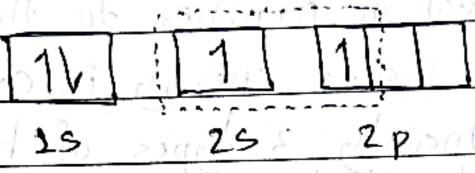
Formation of BeF_2 molecule

The central atom Be in BeF_2 undergoes sp ~~hydrilizat~~ hybridization to give two half filled sp orbitals which are linearlly arranged. Each half-filled sp- ~~ort~~ hybrid orbital of Be atom mutually share electron with half filled p-orbital of two ~~fe atom~~ Fluorine atom to give BeF_2 ~~ato~~ molecule. Hence, form molecule has linear geometry with bond angle 180°.

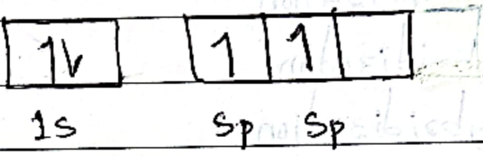
Ground state :



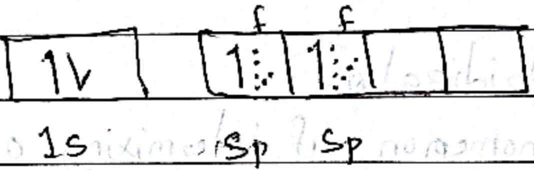
Exicted state (E.s) :



~~Hybri~~ SP-hybridization :



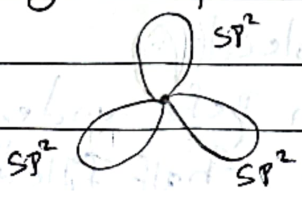
In BeF_2 molecule :



ii. Sp^2 Hybridization

The phenomenon of intermixing one s-orbital and two p-orbitals with comparable energy of an atom to give three hybrid orbitals having the identical shape and the same energy content is called Sp^2 ~~hyd~~ hybridization.

Each sp^2 hybrid orbital has its 33.3% s-charactor and 66.6% P-character. To minimise the repulsion, they are directed towards three corners of an equilateral triangle. So the shape of the molecule whose central atom undergoes sp^2 hybridization is trigonal planar.



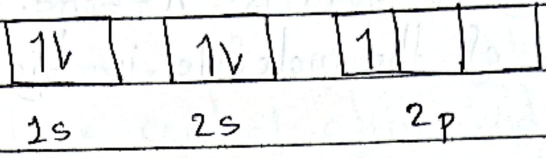
Trigonal Planar shape

Formation of BCl_3 molecule

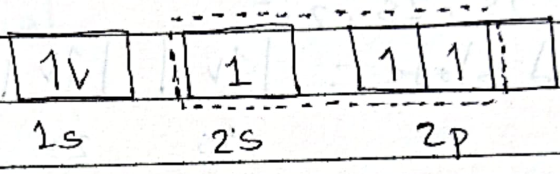
The central atom Boron in BCl_3 undergoes sp^2 hybridization to form 3 half filled sp^2 hybrid orbitals. Each half-filled sp^2 orbitals mutually share electron with 3 chlorine atom by sigma covalent bond to give BCl_3 molecule. Hence formed molecule has trigonal planar geometry with bond angle 120°.

$B = 1s^2, 2s^2, 2p^1$

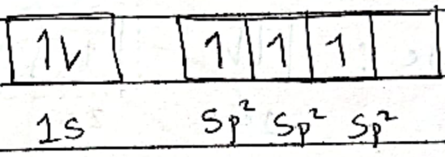
Ground state E.C :



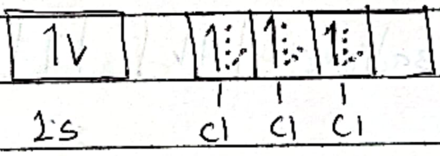
Excited state E.C. :



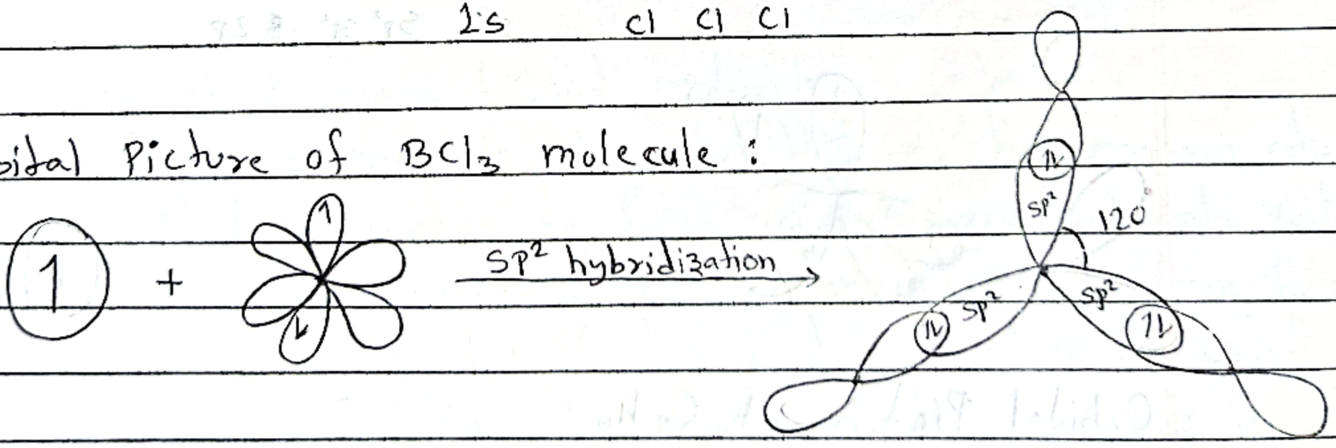
Sp^2 hybridization :

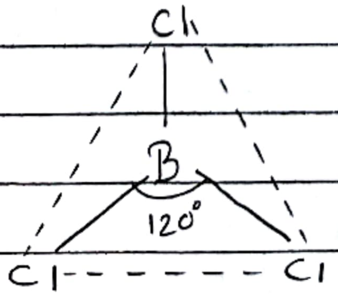


In BCl_3 molecule :



Orbital Picture of BCl_3 molecule :





Trigonal planar geometry

Bonding structure of BCl_3

Formation of Ethene (C_2H_4) molecule

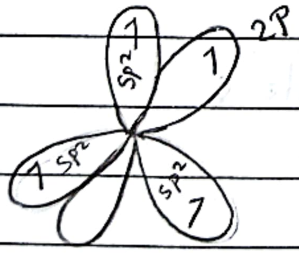
In an ethene molecule, orbitals of carbon atom undergoes sp^2 hybridization to form three hybrid orbitals having the identical shape and the same energy ~~level~~ content. They form 2 σ-bond with 1s orbitals of the hydrogen atom and 1 σ-bond with a hybrid orbitals of another carbon atom. The pure p-orbitals of each carbon atom undergoes sidewise overlapping to form a π-bond. Since there is sp^2 hybridizati the shape of the molecule is trigonal planar.

$C = 1s^2, 2s^2, 2p^2$

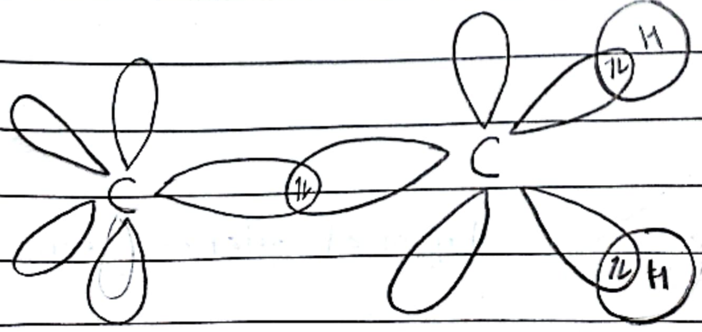
Ground state : [↑↓] [↑↓] [↑|↑|]
1s 2s 2p

Excited state : [↑↓] [↑] [↑|↑|↑]
1s 2s ~~sp~~ 2p

sp^2- hybridization: [↑↓] [↑|↑|↑|↑]
sp^2 sp^2 sp^2 2p



Orbital Picture of C_2H_4

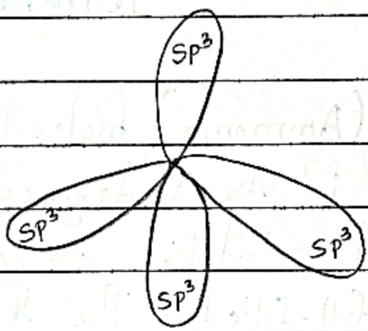


iii. Sp^3 Hybridization

The phenomenon of intermixing one s-orbital and three p-orbital with comparable energy of an atom to give for hybrid orbitals having identical shape and same energy content is called sp^3 hybridization.

E

Each hybrid orbital has 25% s-character and 75% p-character. To minimise the repulsion between them, they are directed towards four corners of regular tetrahedral. So the shape of a molecule whose central atom undergoes sp^3 hybridization is tetrahedral.



Tetrahedral shape

Formation of Methane (CH_4) molecule

To form methane molecule, the orbitals of the carbon atom undergo sp^3 hybridization to form four hybrid orbitals with identical shape and the same energy content. They form four σ-bond with 1s orbital of the hydrogen atom. Since there is sp^3 hybridisation, the shape of the molecule is tetrahedral.

$C = 1s^2, 2s^2, 2p^2$

Ground state:

↑↓	↑↓	↑	↑	
1s	2s	2p		

Excited state:

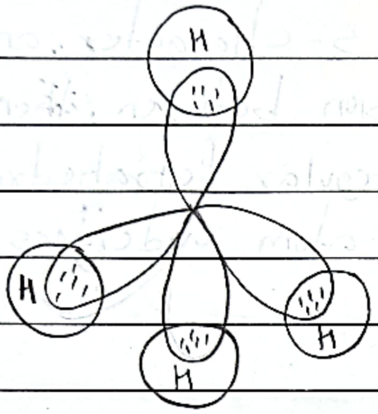
↑↓	↑	↑	↑	↑
1s	2s	2p		

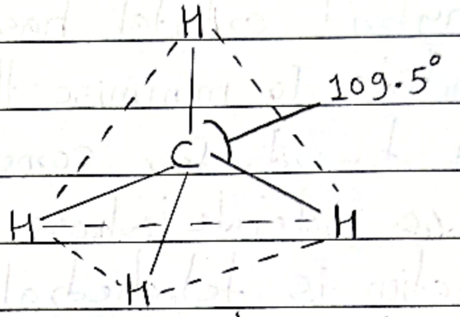
Sp^3 hybridization : ↑↓ ↑ ↑ ↑ ↑

1s Sp^3

In CH_4 : ↑↓ ↑⁝ ↑⁝ ↑⁝ ↑⁝

H H H H





Tetrahedral shape

Formation of NH_3 (Ammonia) molecule

The central atom N in NH_3 undergoes sp^3 hybridization do give four sp^3 hybrid orbitals. Among them three are half filled and one is full-filled. The three half filled sp^3 hybrid orbitals of nitrogen mutually share electron with 3 hydrogen atoms to give NH_3 molecule. The expected geometry of NH_3 is tetrahedral but due do repulsive intraction between a lone pair of electron and bond pair of electron the actual geometry of NH_3 is distorted tetrahedral or pyramidal with bond angle 107.5°

$N = 1s^2, 2s^2, 2p^3$

Ground state : ↑↓ ↑↓ ↑ ↑ ↑

1s 2s 2p

Exicted state : ↑↓ ↑ ↑↓ ↑ ↑

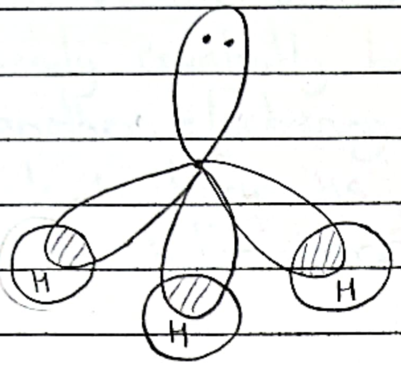
1s 2s 2p

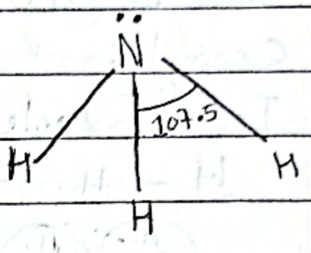
sp^3 hybridization : |↑↓| |↑↓|↑|↑|↑|

sp^3 sp^3 sp^3

In NH_3 : |↑↓| |↑↓|↑↓|↑↓|↑↓|

H H H





Pyramidal shape

Dipole Moment (μ)

It is defined as the product of the magnitude of charge developed in an atom of a molecule and the distance between the combining atom. It is denoted by μ i.e. $\mu = q \cdot d$. It, is a vector quantity. Its value depends upon the geometry of the molecule. It is the resultant of the dipole moment of all the bonds involved in the molecule. Its unit is Debye (D).

If the dipole moment of the molecule is zero, the molecule is said to be non-polar. If the dipole moment of a molecule is greater than zero, the molecule is said to be polar.

Application of dipole moment

i. To predict the polar or non-polar molecules
ii. To predict the shape of the molecule.
iii. Gives an idea about the degree of polarity or ionic character of molecules.

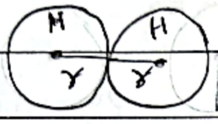
Bond Length

The distance between the nuclei of two bonded atom is called bond length. For homo-atomic molecule like H_2, O_2, Cl_2 etc. the bond length is doubled to their atomic radii and in case of hetero-atomic molecule the bond length is the sum of the radius of bonded atoms.

Example:

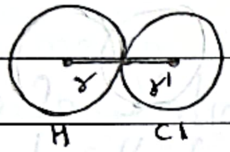
In H_2 molecule

$H - H = 0.74$



$l = r + r = 2r$

In HCl molecule



$l = r + r'$

Ionic Character

The development of positive and negative pole in a covalent molecule / bond due to unsymmetrical distribution of electron is called ionic character. It depends upon two main factors;

i. The electronegativity difference of bonded atom and

ii. Dipole moment of polar molecule.

The amount of ionic character in a polar covalent bond depends upon the difference of electronegativity of bonded atom. Greater is the value of electronegativity difference, higher will be the percentage of ionic character in the polar covalent bond.

The percentage of ionic character can be determined from the ratio between experimental and theoretical value of dipole moment

$$\text{Ionic Character} = \frac{\text{Exp. value of dipole moment}}{\text{Theor. value of dipole moment}} \times 100$$

Hydrogen Bonding and It's Application

The electrostatic attraction between a hydrogen atom which is already covalently bonded with an electronegative atom and another electronegative atom of same or different molecule is known as hydrogen bond. For example:

$$H^{\delta+} — Cl^{\delta-} \cdots\cdots H^{\delta+} — Cl^{\delta-}$$

Hydrogen Bond

Types of Hydrogen Bonding

i. Inter-molecular H-Bonding

Hydrogen bond formed between hydrogen atom of one molecule and electronegative atom of another molecule is called inter molecular hydrogen bonding or polymerization.

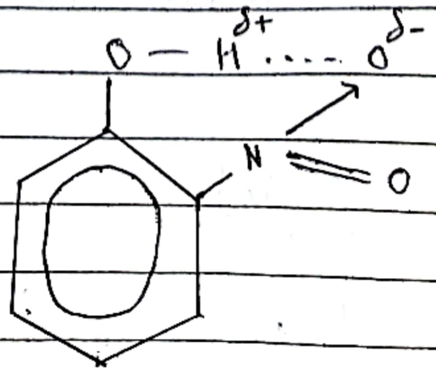
For example:

$$H^{\delta+} — F^{\delta-} \cdots H^{\delta+} — F^{\delta-} \cdots H^{\delta+} — F^{\delta-} \cdots H^{\delta+} — F^{\delta-}$$

ii. Intra-molecular Hydrogen Bonding

The hydrogen bond formed between a hydrogen atom and a highly electronegative atom present in the same molecule is called intra-molecular hydrogen bonding or chelate ring.

For example:



Application of Hydrogen Bonding

i. Due to inter-molecular H-bonding water exist in liquid state.

ii Due to inter-molecular H-bonding formation of macro molecule is possible.

iii. Wood, fibre are rigid ~~due to H~~ due to H-bonding.

iv. The rigidity and tensile strength of cotton silk.

Metallic Bonding

The force of attraction among the particles of metal is called a metallic bond. According to the electron gas model, it is the force of attraction between the mobile electron and positively charged kernals (a portion of atom left after the loss of electron).

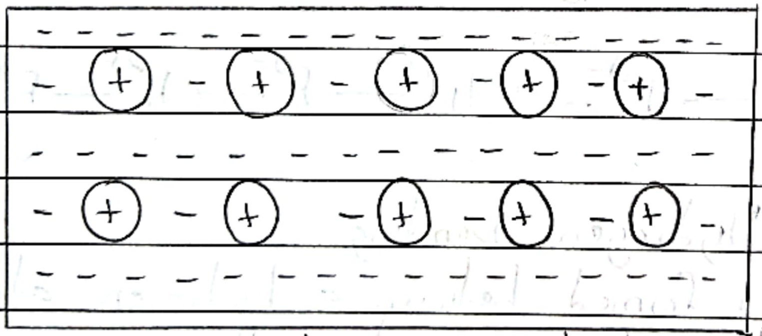


Fig: Electron sea model of metallic bond.

The force of attraction between mobile electrons and positively charged kernels which holds metal atoms together is called metallic bond

Characteristics of Metal

i. Electrical Conductivity

Due to presence of mobile electrons around the kernels of metal they can easily conduct electricity or metal are good conductors.

ii. Thermal Conductivity
On heating metals, the mobile electron absorbs heat energy and increase their vibrational motion so that the heat is conducted throughout the metal. Hence, metal are ~~good thermally~~ thermally conducting material.

iii. Metallic Lustre
When light falls on the surface of metal, the electron absorbs the light and moves to exicted state where they are unstable and return to ground state emitting light radiation so that the surface of metal looks shiny which is called metallic lustre.

iv. Malleability and Ductility
Due to strong metallic bonding, metals are converted ~~to~~ into thin sheet on beating which is called malleability and if metal pieces are drawn forcely they converted into wire which is called ductility.

Vander Waal's Force of attraction
The intermolecular (inter-atomic) short-lived attractive force which is able to holds atom, molecules or ions close to each other is called vander Waal's force of attraction.
This types of force is quite difference from purely electro-static force that exist between ~~a posit~~ oppositively charged ions or the force that holds atom together through covalent bond.

It is an Instantaneous force of attraction which is weaker than a hydrogen bond. It increase with increasing surface area of the molecule and increasing polarity ~~of~~ in the molecule.

Types of Van der Waal's force

i. Dipole - dipole interaction : It exists among polar molecules like HCl, HBr, H_2O etc.

ii. Ion-dipole interaction (Debye force) : It exists among ion and polar compounds. eg: a force of attraction between NaCl and H_2O.

iii. Instantaneous dipole - induced dipole interaction : It occurs between non-polar molecules like, Ar, He, Cl_2, CH_4 etc.

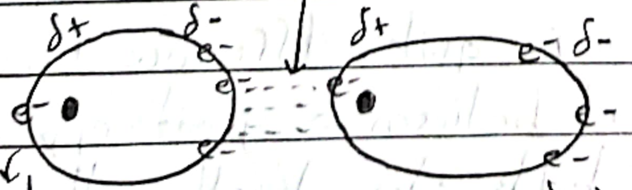
Applications of Van der Waal's force

i. This force is responsible for the solidification and liquificatio of inert gas and some other gases.

ii. Soft crystalline solid having low melting point are held together by Van der Waal's force of attraction.

iii. This force has major role in the field of structural biology, polymer science, nano technology and Surface ~~technology~~ science.

Vander Waal's force of attraction



Induced dipole
caused by instataneous dipole

Instantaneous dipole
caused by external force