CHEMICAL BOND

Prepared by

Shreemoyee Phukan, Silapathar College

A chemical bond is a sort of attraction which keeps the two atoms together. Thus, depending upon the variety of force, there may be variety of chemical bonds.

REASONS FOR THE FORMATION OF A CHEMCIAL BOND:

Energy concept: When two atoms approach each other, the attractive and repulsive forces operate between them. The distance at which the attractive forces overweigh the repulsive forces is known as the bond distance, the potential energy of the system is minimum and the bond is said to be formed.

Lewis and Langmuir: Concept of stable electronic configuration.

Atoms enter into chemical bonding to acquire the stable inert gas electronic configuration. They can do so by losing, gaining or sharing of electrons.

TYPES OF CHEMCIAL BOND

Depending upon the mode of acquiring the stable electronic configuration, the chemical bonds may be

Ionic or electrovalent bond

Covalent bond

Coordinate or dative bond

Metallic bond

Hydrogen bond

Weak van der Waals forces of attraction

IONIC BOND

Ionic bond is formed by the complete transference of one or more valence electrons of one atom to the valence shell of the other atom. Both atoms are converted into ions and have the electronic configuration of nearest noble gases. The ions, which always tends to decrease the potential energy of the system is known as the ionic bond. Consider the formation of KCl. The electronic configuration of K, Cl and their ions (K+ and Cl-) are given below

K (19): $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^1$

K+(18): $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6$ Inert gas (Ar) configuration

Cl (17): $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^5$

Cl$^-$(18): $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6$ Inert gas (Ar) configuration

K$^+$ + Cl$^-$ = KCl

The number of electrons lost or gained by an atom represents the electrovalency of the atom.

FAJAN'S RULE:

This rule is for covalent character of an ionic bond. Covalent character of an ionic bond is favoured by

   Smaller positive ion   (ii) Large negative ion   (iii) Large charge on ions

Thus for a fixed cation, the larger the size of anion, the more the magnitude of the charge, the more is covalent character eg. Covalent character of sodium halides follows the order.

    NaI > NaBr > NaCl > NaF
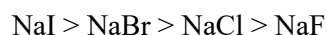
For fixed anion, the smaller the size of cation, the more the magnitude of the charge, the more is the covalent character.

Eg. $BeCl_2$ > $MgCl_2$ > $CaCl_2$ > $SrCl_2$ > $BaCl_2$
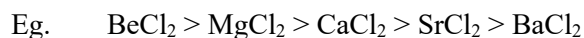
It has been observed that a cation having 18 ($s^2p^6d^{10}$) electrons in outermost shell (pseudo noble gas configuration) can polarize the anion more than cation having 8 (s^2p^6) noble gas electronic configurations. Hence CuCl is more covalent than NaCl. Similarly AgCl is more covalent that KCl.

POLARISING POWER OF CATION :

The power of cation to attract the electron cloud toward itself is called polarizing power of cation.

POLARISATION:

When cation and anion come closer to each other, the electron could of anion is attracted towards the cation; some partial sharing of electrons take place, the anion is distorted and the effect is known as polarisation.

*More the effect of polarisation, more is the sharing of electrons and the more is covalent character of ionic bond.
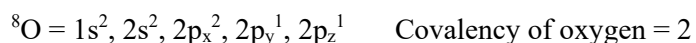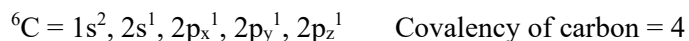
COVALENT BOND:

According to G.N. Lewis, atoms may also combine by sharing of electrons in their outermost shells and attain noble gas electronic configuration. One shared pair of electrons constitute a single bond, two electron pairs constitute a double bond so on. The bonds thus formed are known as covalent bonds.
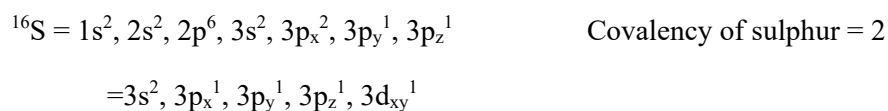
COVALENCY:

It is the number of electron pairs shared by one atom of the element in combination with other atoms in a molecule. It can also be defined as the number of covalent bonds formed by the atom of the element with other atoms.
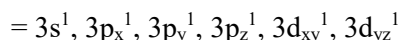
Variable Covalency:

Generally the covalency of an element is equal to the total number of unpaired electrons in s and p orbitals of the valence shell. For example

$^6C = 1s^2, 2s^1, 2p_x^1, 2p_y^1, 2p_z^1$ Covalency of carbon = 4

$^8O = 1s^2, 2s^2, 2p_x^2, 2p_y^1, 2p_z^1$ Covalency of oxygen = 2

❖ The variable covalency is shown by elements having vacant d-orbitals in their valence shell. The unpairing of the s and p electrons is possible by promoting them to d-orbitals. For example

$^{16}S = 1s^2, 2s^2, 2p^6, 3s^2, 3p_x^2, 3p_y^1, 3p_z^1$ Covalency of sulphur = 2

       $= 3s^2, 3p_x^1, 3p_y^1, 3p_z^1, 3d_{xy}^1$

First excited state   covalency of sulphur = 4

       $= 3s^1, 3p_x^1, 3p_y^1, 3p_z^1, 3d_{xy}^1, 3d_{yz}^1$

Second excited state   covalency of Sulphur = 6

Similarly, other than fluorine, the halogens have high covalencies equal to 3, 5 and 7. Phosphorous shows covalencies equal to 3 and 5.

The elements having no d-orbitals do not exhibit variable covalency.

NATURE OF COVALENT BOND

The nature of covalent bond is explained by

➢ Heitler – london theory
➢ Pauling – slater theory
➢ Hund – mulliken theory
➢ Valence bond theory
➢ Molecular orbital theory

VALENCE BOND THEORY: This theory is given by Heiteler and London, to explain how a covalent bond is formed. This theory is explained by a Slater, the main points of this theory are;

A covalent bond is formed by the overlapping between two half filled atomic orbitals having electrons with opposite spin.

The atom with half fill atomic orbitals comes closer to one another at a proper axis.

As a result of overlapping, there is maximum electron density between the two atoms.

Greater the overlapping, higher is the strength of chemical bond.

Two types of bonds are formed on account of overlapping. These are-

 (a) Sigma bond (σ) and (b) Pi bond (π).

Sigma bond (σ bond) – This type of covalent bond is formed by the end to end overlapping of orbitals along the inter-nuclear axis. The overlap is known as head on overlap or axial overlap. The following overlapping result in the formation of sigma bond.

s – s overlapping (Formation of Hydrogen Molecule)

s – p overlapping (Formation of HF, HCl Molecules)

p – p head on overlapping (Formation of F_2, Cl_2 Molecules)

Bond between two hybrid orbitals sp^3-sp^3, sp^2-sp^2, sp^3-sp^2, sp^3-sp, sp^2-sp, sp-sp etc. overlapping of orbitals form σ bond.

pi – bond (π - bond) – It is formed by the sidewise or lateral overlapping between unhybridised p – atomic orbitals. The orbitals involved in side wise overlap must be parallel and perpendicular to the inter-nuclear axis. It is always accompanied by a σ bond and consist of two charge clouds i.e. above and below the plane of sigma bond.

Since overlapping take place on both sides of the inter-nuclear axis free rotation of atoms around a pi bond is not possible.

- π bond is a weaker bond than σ - bond.

The strength of σ-bond depends upon the extent of overlapping between atomic orbitals. Greater the overlapping stronger is the σ - bond. It follows the following order

- s – s > s – p > p – p
- Single bond is always σ- bond.
- In multiple bonds only one is σ bond, others are π-bonds.
- π-bond is not formed by hybrid orbitals.

LIMITATIONS OF VALENCE BOND THOERY:

- It fails to explain the magnetic properties of some molecules.
- Bonding in electron deficient compounds.
- It could not define the formation of H2+
- It could not explain the paramagnetic character O2.
- It could not explain the formation of Coordinate bond.
- It could not explain the Fazan's Rule.

Differences between Valnce Bond Theory (VBT) and Molecular Orbital Theory(MOT)

Valence Bond Theory	Molecular Orbital Theory
1. Electrons in the molecule are localized as if they are in isolated atoms.	It regards the nuclei of the molecules as polycentric and then constructs the molecule.
2. The atomic orbitals of the combining atoms retain their individual identity to large extent.	The atomic orbitals of the combining atoms lose their individual identity in the molecular orbitals.
3. It takes into account only the increase in the electron density in the region of orbital overlap.	It takes into account the increase as well as decrease in electron density in the region of orbital overlap.
4. The number of covalent bonds formed is equal to half of the number of combining atomic orbitals .	The number of bonds (or bond order) is half the difference in the bonding and antibonding electrons.
5. It does not predict the paramagnetic or diamagnetic behavior of molecules or ions.	It can predict the paramagnetic and diamagnetic behavior of molecules or ions.
6. It is quite easy to apply.	
7. Resonance has an important role in this theory.	It is rather difficult to apply.
	Resonance has no role in this theory.

MOLECULAR ORBITAL THEORY OR HUND-MULLIKEN THEORY:

According to this theory the atomic orbitals combine to form the molecular orbitals. The number of molecular orbitals formed is equal to the number of atomic orbitals involved and they belong to the molecule.

The molecular orbitals are formed by LCAO method (linear combination of atomic orbitals) i.e. by addition or subtraction of wave functions of individual orbitals thus

Molecular orbital of lower energy is known as bonding molecular orbital and of higher energy is known as antibonding molecular orbital.

Molecular orbitals are characterized by a set of quantum numbers.

Bond order- It is defined as one half the difference between the number of electrons present in the bonding and the antibonding orbitals.

i.e. Bond order (b.o) = ½ (N_b – N_a). where, N_b=no. of bonding electrons

N_a=no. of antibonding electrons

Stability of molecule- bond order.

The bond order of 1, 2 and 3 corresponds to single, double and triple bond respectively. It may be mentioned that according to M. O. theory, even a fractional bond order is possible.

Magnetic property – If all the elements in a molecule are paired then substance is diamagnetic, on the other hand if there are unpaired electrons in the molecule the substance is paramagnetic. More the number of unpaired electrons in the molecule greater is the paramagnetism of the substance.

ELECTRONIC CONFIGURATION/ BOND ORDER OF SIMPLE DIATOMIC MOLECULES:

The electronic configuration and the bond order in case of simple diatomic molecules can be obtained by filling the molecular orbitals by applying Aufbau principle and Hunds rule. The increasing order of energies of various molecular orbitals upto N_2 molecule is

$\sigma_{1s} < \sigma_{1s}* < \sigma_{2s} < \sigma_{2s}* < (\pi_{2px} = \pi_{2py}) < \sigma_{2pz} < (\pi_{2px}* = \pi_{2py}*) < \sigma_{2pz}*$

For O_2 and F_2 is given below

$\sigma_{1s} < \sigma_{1s}* < \sigma_{2s} < \sigma_{2s}* < \sigma_{2pz} < (\pi_{2px} = \pi_{2py}) < (\pi_{2px}* = \pi_{2py}*) < \sigma_{2pz}*$

Sl. No	Molecule/ ion	No. of electrons	Electronic Configuration	Bond Order ½ (N_b – N_a)	Magnetic Property
1	H_2	2	$(\sigma 1s)^2$	½ (2 – 0)=1	Diamagnetic
2	H_2^+	1	$(\sigma 1s)^1$	½ (1 – 0)=1/2	Paramagnetic
3	H_2^-	3	$(\sigma 1s)^2 (\sigma^* 1s)^1$	½ (2 – 1)=1/2	Paramagnetic
4	He_2	4	$(\sigma 1s)^2 (\sigma^* 1s)^2$	½ (2 – 2)=0	Does not exist
5	He_2^+	3	$(\sigma 1s)^2 (\sigma^* 1s)^1$	½ (2 – 1)=1/2	Paramagnetic
6	B_2	10	$(\sigma 1s)^2 (\sigma^* 1s)^2(\sigma 2s)^2(\sigma^* 2s)^2(\pi 2p_x^1 = \pi 2p_y^1)$	½ (6 – 4)=1	Paramagnetic
7	C_2	12	$(\sigma 1s)^2 (\sigma^* 1s)^2(\sigma 2s)^2(\sigma^* 2s)^2(\pi 2p_x^2 = \pi 2p_y^2)$	½ (8 – 4)=2	Diamagnetic
8	N_2	14	$(\sigma 1s)^2(\sigma^* 1s)^2(\sigma 2s)^2(\sigma^* 2s)^2(\pi 2p_x^2 = \pi 2p_y^2)(\sigma 2p_z^2)$	½ (10 – 4)=3	Diamagnetic
9	N_2^+	13	$(\sigma 1s)^2(\sigma^* 1s)^2(\sigma 2s)^2(\sigma^* 2s)^2(\pi 2p_x^2 = \pi 2p_y^2)(\sigma 2p_z^1)$	½ (9 – 4)=5/2	Paramagnetic
10	O_2	16	$KK(\sigma 2s)^2(\sigma^* 2s)^2(\sigma 2p_z^2)(\pi 2p_x^2 = \pi 2p_y^2) (\pi^* 2p_x^1 = \pi^* 2p_y^1)$	½ (10 – 6)=2	Paramagnetic

11	O_2^+	15	KK $(\sigma 2s)^2(\sigma^*2s)^2(\sigma 2p_z)^2(\pi 2p_x^2 = \pi 2p_y^2)(\pi^*2p_x^1 = \pi^*2p_x^0)$	½ (10 − 5)=2.5	Paramagnetic
12	O_2^-	17	KK $(\sigma 2s)^2(\sigma^*2s)^2(\sigma 2p_z)^2(\pi 2p_x^2 = \pi 2p_y^2)(\pi^*2p_x^2 = \pi^*2p_y^1)$	½ (10 − 7)=1.5	Paramagnetic
13	O_2^{2-}	18	KK$(\sigma 2s)^2(\sigma^*2s)^2(\sigma 2p_z)^2(\pi 2p_x^2 = \pi 2p_y^2)(\pi^*2p_x^2 = \pi^*2p_y^2)$	½ (10 − 8)=1	Diamagnetic
14	F_2	18	KK LL $(\sigma 2p_z)^2(\pi 2p_x^2 = \pi 2p_y^2)(\pi^*2p_x^2 = \pi^*2p_y^2)$	½ (10 − 8)=1	Diamagnetic
15	NO	15	KK $(\sigma 2s)^2(\sigma^*2s)^2(\sigma 2p_z)^2(\pi 2p_x^2 = \pi 2p_y^2)(\pi^*2p_x^1 = \pi^*2p_y^0)$	½ (10 − 5)=2.5	Paramagnetic
16	CO	14	$(\sigma 1s)^2(\sigma^*1s)^2(\sigma 2s)^2(\sigma^*2s)^2(\sigma 2p_z)^2(\pi 2p_x^2 = \pi 2p_y^2)$	½ (10 − 4)=3	Diamagnetic

HYBRIDISATION:

Hybridisation is the redistribution of energy levels at the time of formation of molecules. It may also be defined as intermixing of atomic orbitals of nearly the same energy and resulting in the formation of new atomic orbitals same in number and identical in all respects (shape, energy and size). The new atomic orbitals are known as hybrid atomic orbitals.

The completely filled or half filled atomic orbitals can take part in hybridization and hybrid atomic orbitals form stronger bonds.

sp^3 Hybridization. If one s and three p-orbitals are intermixed or hybridized, this is known as sp3-hybridization. Four equivalent orbitals will be formed which are called sp^3 hybridized orbitals which are directed along the four corners of a tetrahedron with bond angle 109° 28′, e.g., in CH_4, carbon undergoes sp^3 hybridization and it has tetrahedral shape.

sp^3d Hybridisation. When one s, three p and one d-orbitals intermix together and give rise to five sp^3d hybridized orbitals. The shape of molecule is trigonal bipyramidal. Bond angle is 90°, 120°, e.g., PF_5, PCl_5 involves sp^3d hybridization.

sp^3d^2 Hybridisation. When one s, three p and two d-orbitals intermix to give rise to six sp^3d^2 hybridised orbitals. The shape of molecule having sp^3d^2 hybridisation will be octahedral with bond angle 90°, e.g., SF_6, involve sp^3d^2 hybridisation and possess octahedral shape.

sp^2 Hybridisation. If one s and two p-orbitals are intermixed, it is called sp^2-hybridization. Three equivalent orbitals are called sp2 hybridized orbitals which will be directly along the corners of equilateral triangle having bond angle 120°, e.g., in BF_3, 'B' atom undergoes sp^2 hybridization and its shape is a planar.

sp Hybridisation. If one s and one p orbital intermix, it is called sp-hybridization. The two sp hybridized orbitals are far-apart. In BeF_2, Be atom undergoes sp-hybridization and it has linear shape with bond angle 180°.

**Hybridisation in some important molecules.**

CH$_4$ molecule. C (6) has electronic configuration in ground state 1s^2 2s^2 2p$_x$^{1} 2p$_y$^{1}2p$_z$^{0} C (6) in excited state 1s^{2}2s^{1}2p$_x$^{1}2p$_y$^{1}2p$_z$^{1}(since carbon is tetravalent we need excited state).

2S   2p

| ↑ | | ↑ | ↑ | ↑ |

2S   ←——2p——→

| ↑ | | ↑ | ↑ | ↑ |
  H   H   H   H

sp3 hybridization
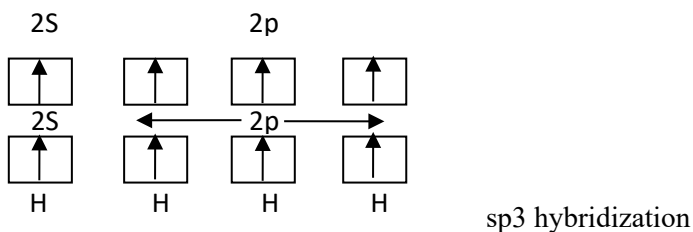
- **NH$_3$ molecule**. N(7) 1s^{2}2s^{2}2p$_x$^{1}2p$_y$^{1}2p$_z$^{1} (since nitrogen is trivalent we do not need excited state).

| ↑↓ | | ↑ | ↑ | ↑ |

2S   ←——2p——→

| / | | / | / |
  H   H   H
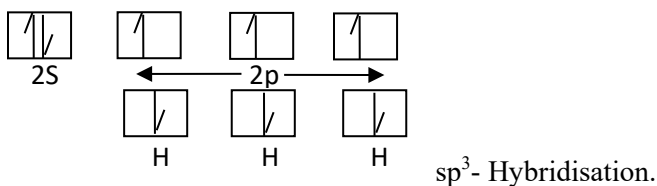
sp^3- Hybridisation.

- **H$_2$O molecule.** O (8) 1s^{2}2s^{2}2p$_x$^{2}2p$_y$^{1}2p$_z$^{1} (since oxygen is divalent, we do not need excited state).

2S   2p

| ↑↓ | | ↑↓ | ↑ | ↑ |

2S   ←——2p——→

| / | | / |
  H   H
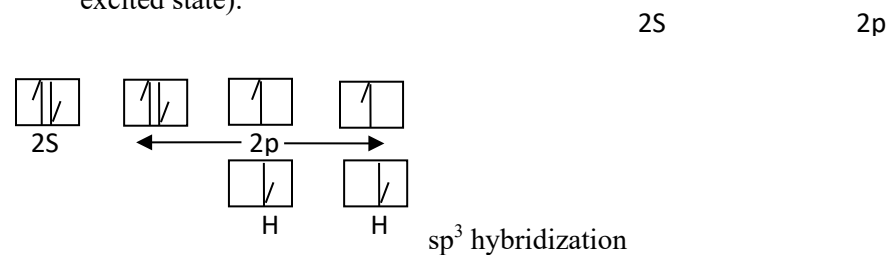
sp^3 hybridization

(i) **sp^2- Hybridisation.**
   BF$_3$ molecule. B(5) 1s^{2}2s^{2}2p$_x$^{1} in ground state

B(5): 1s^{2}2s^{1}2p$_x$^{1}2p$_y$^{1}2p$_z$^{0} in excited state (since boron is trivalent only in excited state).

➢   Sp^2 hybridization

METHOD FOR FINDING THE TYPE OF HYBRIDISATION:

Apply the following formula to find the hybridization of central atom.

$$\frac{1}{2}\left(\begin{array}{l} number\ of\ valence\ electrons\ of\ central\ atom \\ +\ number\ of\ monovalent\ atoms\ attached\ to\ it \\ +\ negative\ charge\ if\ any - positive\ charge\ if\ any \end{array}\right) = z$$

Value of z	2	3	4	5	6	7
Hybridisation	sp	sp^2	sp^3	sp^3d	sp^3d^2	sp^3d^3

Examples:

i) Hybridisation of $NH_3 = \frac{1}{2}[5 + 3 + 0 - 0] = 4; sp^3$

ii) Hybridisation of $H_2O = \frac{1}{2}[6 + 2 + 0 - 0] = 4; sp^3$

iii) Hybridisation of $SO_3 = \frac{1}{2}[6 + 0 + 0 - 0] = 3; sp^3$

iv) Hybridisation of $SO_4^{2-} = \frac{1}{2}[6 + 0 + 2 - 0] = 4; sp^3$

v) Hybridisation of $CO_3^{2-} = \frac{1}{2}[4 + 0 + 2 - 0] = 3; sp^2$

vi) Hybridisation of $PCl_3 = \frac{1}{2}[5 + 5 + 0 - 0] = 5; sp^3d$

Hybridisation of $SF_6 = \frac{1}{2}[6 + 6 + 0 - 0] = 6; sp^3d^2$

Polar And Non Polar Covalent Bonds:

If the two bonded atoms have equal values of electronegativites, the bonded pair of electrons is equally shared between them, i.e. shared pair of electrons remains in the middle (just in between the atoms). Such a bond is called non polar covalent bond.

For example H – H, O = O, N = N, C – C, F – F ……………etc bonds. However, if the bonded atoms differ in their electronegativites, the bonded paired of electron is attracted more towards atom with the larger electronegativity, resulting in the development of partial negative charge over this atom and equal but opposite charge over the other bonded atom. Such a covalent bond is called Polar covalent bond.

For e.g. I – Cl, C – Cl, C = O, H – F, H – Cl etc.

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

(non polar molecules)   (polar molecule)

Extent of polarity in a bond is measured in terms of dipole moment.

Dipole Moment (μ): It can be defined as the product of the magnitude of the charge and the distance between the centres of positive and negate e charge. It is usually designed by a Greek letter '□. Mathematically, it is expressed as follows:

Dipole moment (μ) = charge (Q) x distance of separation (r).

Dipole moment is usually expressed in Debye units (D). The conversion factor is

$$1D = 3.33564 \times 10^{-30} \text{ cm}$$

Where C is coulomb and m is meter.

Further dipole moment is a vector quantity and is depicted by a small arrow with tail on the positive centre and head pointing towards the negative centre. For example the dipole moment of HF may be represented as:

$$H^{\delta+}\!\!-\!\!F^{\delta-}$$
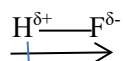
The shift in electron density is symbolised by crossed arrow ($\longmapsto$) above the Lewis structure to indicate the direction of the shift.

Co-ordinate Covalent Bond or Dative Bond:

When both the electrons for sharing between two atoms are contributed by one atom only the bond formed is known as coordinate bond or dative bond.

In terms of orbital theory the co-ordinate covalent bond is formed by overlapping between empty and completely filled atomic orbitals.

The atom donating the pair of electrons is called donor and the atom which accepts the pair of electrons is called acceptor. The compound containing coordinate bonds are known as

co-ordination compounds. The bond is represented by an arrow ($\longrightarrow$) pointing head towards the acceptor.

Once the coordinate bond is formed it is indistinguishable from a covalent bond.

E.g.

$$\overset{\bullet\bullet}{NH_3} + BF_3 \longrightarrow \overset{+}{NH_3}\!\!\longrightarrow\!\!\overset{-}{BF_3}$$

(donor)   (acceptor)
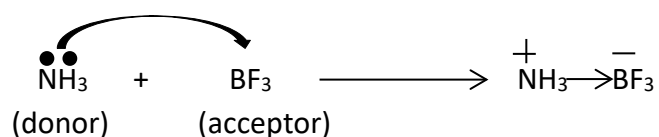
CHARACTERISTICS OF CO-ORDINATE COMPOUNDS:

Co-ordinate compounds have volatile character in between ionic and covalent compounds. Other properties like solubility, electrical conductivity and stereo isomerism are similar to covalent compounds.

HYDROGEN BOND:

It may be defined as the force of attraction existing between hydrogen atom covalently bonded to highly electronegative atom (N, O or F) and the electro negative atom belonging to another molecule of the same or different substance. It is represented by dotted lines (……..).

Hydrogen bond is purely electrostatic in nature. It is a weak bond, the strength of the strongest being about 5 – 10 kcal per mole. The more the electronegativity of atom involved in H – bonding, the more is the bond strength
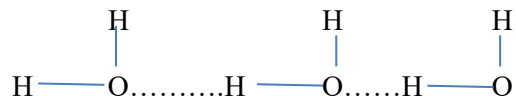
e.g.,

H…F   >   H…O   >   H…N

10 kcal/mole   >   7 kcal/mole > 2.0 kcal/mole

Types of hydrogen bonds – Hydrogen bond is of two types

　　　Intermolecular H-bonding (Association). It is formed between two different molecules of the same of different substances. For example
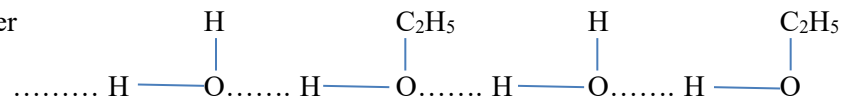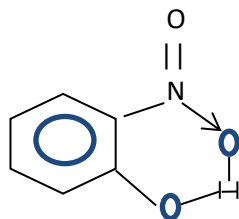
HF

H——F……H —— F…….H —— F

H_2O

Alcohol in water

　　　Intramolecular H – bonding (chelation).

H – bonding taking place within single molecule.

(Ortho nitro phenol)

Applications of intermolecular H – bonding.

Water has the lowest molecular weight among the hydrides of group 6 elements yet it has the highest melting and boiling points

	H_2O	H_2S	H_2Se	H_2Te
Melting point	0°C	-85.5°C	-66°C	-51.2°C
Boiling point	100°C	-60.4°C	-41.5°C	+2°C

It is due to intermolecular H – bonding through which water molecules associate

(b)Ice has less density than water – In crystal structure of ice every water molecule is associated with four other water molecules by H – bonding in a tetrahedral fashion.

It gives rise to cage likes tetrahedral structure of ice with large empty spaces. On melting the ice H – bonds are broken and space between water molecules decreases and density of water increases upto 4°C. Above 4°C more H – bonds are broken, the water molecules move apart from each other and the density again decreases. Thus water has maximum density at 4°C.

(c) Alcohols – The marked difference between the melting and boiling points of alcohols and corresponding mercaptans is also due to association.

	CH_3OH	C_2H_5OH	C_3H_7OH	C_4H_9OH
Boiling point	64.4°C	78°C	97°C	117°C
	CH_3SH	C_2H_5SH	C_3H_7SH	C_4H_9SH
Boiling point	5.8°C	37°C	67°C	97°C

OCTET RULE:

During formation of a covalent bond, the atoms attain an inert gas electronic configuration (ns2p6 configuration). This is known as Octet rule. There are exceptions of octet rule.

Incomplete octet: Examples are $LiCl$, BeH_2 and BCl_3.

Odd-electron molecules: E.g. NO, NO_2

Expanded octet: E.g. PF_5, SF_6, H_2SO_4

Valence Shell Electron Pair Repulsion theory given by Gillespie and Nyholm (VSEPR THEORY)

According to this theory, the bonding and non-bonding electron pairs in the valency shell of the central atom arrange themselves in such a manner that there is minimum repulsion between them. Hence, electron pair orbitals adopt arrangements in space that provide maximum separation among electron pairs.

Following rules should be followed to determine shape of the molecule and bond angle between the atoms:

The molecule which has only bond pair of electrons has definite structure, which provide maximum distance between the bond pairs.

Number of bond pairs	Geometrical distribution of bond pairs	VSEPR notation	Molecular geometry	Bond angle	hybridisation	Example
2	Linear	AB_2	Linear	180°	sp	$BeCl_2$
3	Trigonal planar	AB_3	Trigonal planar	120°	sp^2	BCl_3
4	Tetrahedral	AB_4	Tetrahedral	109.5°	sp^3	CCl_4
5	Trigonal bipyramidal	AB_5	Trigonal bipyramidal	90°, 120°	sp^3d	PCl
6	Octahedral	AB_6	Octahedral	90°	sp^3d^2	SF_6
7	Pentagonal bipyramidal	AB_7	Pentagonal bipyramidal	90°, 72°	sp^3d^3	IF_7

(i) The molecule which has bond pair as well as lone pair of electrons, do not have a definite structure.

(ii) More is the lone pair of electrons, more will be the repulsion and lesser will be the bond angle.

| (iii) Example:	CH_4	NH_3	H_2O
Lone pair of electron(s)	0	1	2
Bond angle	109°28′	107°	104.5
Repulsion	bp – bp <	bp – lp <	lp – lp

lone pair of electrons will distort the geometry of the molecules.

Molecule type	No. of bonding pairs	No. of lone pairs	Arrangement of electron pairs	Shape	Hybridization	Examples
AB_2E	2	1	AB_2	Bent	sp^2	SO_2, O_3
AB_3E	3	1	AB_3E	Trigonal pyramidal	sp^3	NH_3

AB_2E_2	2	2	AB_2E_2	Bent	sp^3	H_2O
AB_4E	4	1	AB_4E	See saw	sp^3d	SF_4
AB_3E_2	3	2	AB_3E_2	T-shape	sp^3d	ClF_3
AB_5E	5	1	AB_5E	Square pyramid	sp^3d^2	BrF_5
AB_4E_2	4	2	AB_4E_2	Square planar	sp^3d^2	XeF_4

RESONANCE

In this case of some of the molecules, all of their properties can't be explained by a single structure. The molecule can be represented by two or more structures. These structures are called canonical forms. The molecule is said to be resonance hybrid of all these structures. These structures have no physical reality in the sense that they cannot be prepared in the laboratory. They exist in imagination. This phenomenon of existing in more than one structure is called resonance, e.g.,
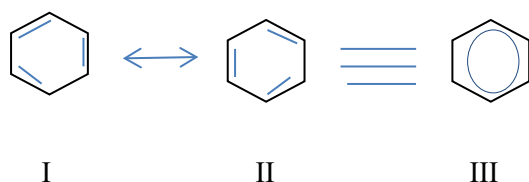
I   II   III

Structures I and II are resonating structure of Benzene and structure III is resonance hybrid of benzene.

RESONANCE ENERGY

It is defined as difference in energy of actual structure of compound and most stable resonating structure, e.g., benzene has resonance energy 150.3 kJ mol^{-1} or 36 kcal mol^{-1}

Note: Draw the resonating structure of the following molecules.

CO_2, CO_3^{2-}, O_3,

Some Important Terms

Lewis structure: Lewis postulated that atoms achieved the stable octet when they were linked by chemical bond. Lewis gave a symbol to denote the valence shell electrons in an atom. The outer shell electrons are shown as dots, surrounding the symbol of the element. It is also known as electron dot symbol. It does not show inner shell electrons.

Example, Na,   • C •

Lattice Enthalpy

The Lattice Enthalpy of an ionic solid is defined as the energy required to completely separating one mole of a solid ionic compound into gaseous constituent ions. For example, the lattice enthalpy of NaCl is 788

kJ mol^{-1}. This means that 788 kJ of energy is required to separate one mole of solid NaCl into one mole of Na$^+$ (g) and one mole of Cl$^-$ (g) to an infinite distance.

BOND LENGTH

Bond length is defined as the equilibrium distance between the nuclei of two bonded atoms in a molecule. Bond lengths are measured by spectroscopic, X-ray diffraction and electron-diffraction techniques.

It is expressed in angstrom (Å) units (1 Å = 10^{-8} cm = 10^{-10} m or pm [(picometer) 1 pm = 10^{-12} m).

In ionic bonds, bond length between two bonded atom is obtained by adding up their ionic radii. The covalent radius is measured approximately as the radius of an atom's core which is in contact with the core of an adjacent atom in a bonded situation. The van der Waals radius represents the overall size of the atom which includes its valence shell in a non-bonded situation.

BOND ANGLE

It is defined as the angle between the orbitals containing bonding electron pairs around the central atom in a molecule/ complex ion. Bond angle is expressed in degree which can be experimentally determined by spectroscopic methods. It gives some idea regarding the distribution of orbitals around the central atom in a molecule/ complex ion and hence it helps us in determining its shape. For example H–O–H bond angle in water is 104.5°.

BOND ENTHALPY

It is defined as the amount of energy required to break one mole of bonds of a particular type between two atoms in a gaseous state. The unit of bond enthalpy is kJ mol^{-1}. For example, the H – H bond enthalpy in hydrogen is 435.8 kJ mol^{-1}.

BOND ORDER

Bond order is the number of bonds between the two atoms in a molecule. For example, in H$_2$ the bond order is 1 since it has single shared electron.