

E-Text in Chemistry

Chapter 4

CHEMICAL BONDING AND MOLECULAR STRUCTURE

The attractive force that binds the atoms together in a molecule is called a chemical bond. It is formed either by the transfer of electrons or by the sharing of electrons.

Lewis symbols

G.N Lewis introduced simple notations to represent valence electrons in an atom. These notations are called Lewis symbols. The symbol of the element and its valence electrons by dots or crosses.

E.g. for sodium [11Na -2,8,1], the Lewis symbol is Na x

and for chlorine [17Cl -2,8,7], the Lewis symbol is $\cdot\ddot{\text{Cl}}\cdot$

Octet rule

According to Lewis and Kossel rule, *atoms undergo chemical reaction in order to attain an octet of electrons in the valence shell.*

Ionic or Electrovalent Bond

A bond formed by the transfer of electron between 2 atoms is called ionic or electrovalent bond.

E.g. formation of NaCl

The factors favouring the ionic bond formation are:

- Low ionisation enthalpy of the electropositive atom (metal atom)
- High negative electron gains enthalpy of the electronegative atom (non-metal atom)
- High lattice enthalpy of the ionic compound formed.

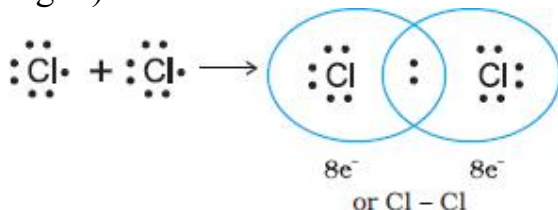
Lattice Enthalpy

It is the energy required to completely separate one mole of an ionic compound into corresponding gaseous ions.

Covalent bond

A bond formed by the mutual sharing of electrons between two or more atoms is called covalent bond.

e.g. 1) The formation of Chlorine molecule (Cl_2)



The covalency of each Cl atoms is one, in O₂ molecule, the covalency is 2 and in N₂ is 3.

Limitations of Octet rule

- 1) It could not explain the stability of compounds containing less than 8 electrons around the central atom. E.g. LiCl, BeH₂, BCl₃
- 2) It could not explain the stability of molecules containing odd number of electrons like NO, NO₂
- 3) It could not explain the stability of molecules containing more than 8 electrons around the central atom (Expanded octet).
E.g. PF₅, SF₆, H₂SO₄, IF₇
- 4) The octet rule is based upon the chemical inertness of noble gases. But some noble gases like xenon and krypton form compounds with F and O.
- 5) This theory does not account for the shape of molecules.
- 6) It does not explain the relative stability of the molecules.

Bond Parameters

- 1) **Bond Length:** It is defined as the average equilibrium distance between the nuclei of two bonded atoms in a molecule. It is expressed in pico-metre (pm) or in angstrom unit (Å⁰).
- 2) **Bond Angle:** It is defined as the angle between the orbitals containing bonding electron pairs around the central atom in a molecule.
- 3) **Bond Enthalpy:** It is defined as the amount of energy required to break one mole of a particular bond between 2 atoms in gaseous state. Its unit is kJ/mol.
- 4) **Bond order:** It is defined as the number of bonds between 2 atoms in a molecule. For H₂, bond order = 1, for O₂, bond order = 2 and for N₂, bond order = 3. *Generally, with increase in bond order, bond enthalpy increases and bond length decreases.*

Resonance Structures

In the case of some compounds, all the observed properties cannot be explained by a single structure. These different structures are called *resonance structures*. The phenomenon is known as *resonance*.

Eg. Resonance structure of Ozone, Benzene

Characteristics of resonance

- Resonance stabilizes the molecule. As the number of resonating structures increases, the stability also increases.
- Resonance changes the bond length.
- The difference in energy between the actual structure and the most stable canonical structure is called resonance energy. Greater the resonance energy, stabler will be the molecule.

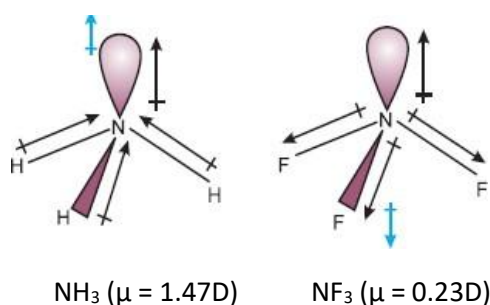
Polarity of bonds : Dipole moment

The polarity of a molecule is expressed in terms of *dipole moment* (μ). It is defined as *the product of the magnitude of charge at one end (Q) and the distance between the charges (r)*.

Mathematically, $\mu = Q \times r$.

The unit of dipole moment is Coulomb metre (Cm). But it is usually expressed in the unit Debye (D). $1D = 3.336 \times 10^{-30} \text{Cm}$.

Eg: The dipole moment of NF_3 is smaller than that of NH_3 . In NH_3 , the orbital dipole due to lone pair is in the same direction as the resultant dipole moment of the three N – H bonds. But in NF_3 , the orbital dipole is in the opposite direction to the resultant dipole moment of the three N-F bonds. So, the dipole moments get partially cancelled.



Covalent character in ionic bonds – Fajans Rules

The partial covalent character of ionic bonds was explained by Fajans rules:

- The smaller the size of the cation and the larger the size of the anion, the greater the covalent character of an ionic bond.
- The greater the charge on the cation, the greater the covalent character of the ionic bond.
- For cations of the same size and charge, the ion with d electronic configuration is more polarizing than the ion with a noble gas configuration.

The Valence Shell Electron Pair Repulsion [VSEPR] Theory

This theory was proposed by Sidgwick and Powell and later modified by Nyholm and Gillespie. The important postulates are:

- 1) The shape of the molecule depends on the number of valence shell electron pairs (VSEPRs) around the central atom.
- 2) The valence shell electron pairs repel each other.
- 3) In order to reduce the repulsion, the electron pairs stay at maximum distance.
- 4) Presence of lone pairs of electron causes distortion in the expected geometry of the molecule.
- 5) The repulsion between two lone pairs of electrons is different from those between two bond pairs or between a lone pair and bond pair. The repulsion decreases in the order lone pair - lone pair > lone pair - bond pair > bond pair - bond pair.
- 6) As the angle between the electron pairs increases, the repulsion decreases.

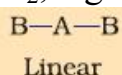
Prediction of geometry of molecules using VSEPR theory

I) Molecules containing only bond pairs of electrons

- 1) **AB₂ type** (where A is the central atom and B is the no. of bond pairs)

Here there are 3 VSEPs. In order to reduce the repulsion, these electron pairs are arranged at an angle of 180°. Thus, the shape of the molecule is linear with bond angle 180°.

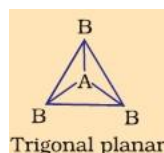
E.g. BeCl₂, HgCl₂



- 2) **AB₃ type**

Here there are 3 VSEPs. In order to reduce the repulsion, these electron pairs are arranged at an angle of 120°. Thus, the shape of the molecule is planar triangular (trigonal planar) with bond angle 120°.

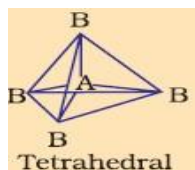
e.g. BF₃, BCl₃



- 3) **AB₄ type**

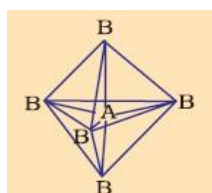
Here there are 4 VSEPs. These are arranged at the four corners of a tetrahedron and hence the shape of the molecule is tetrahedral with bond angle 109°28'.

Eg: CH₄, NH₄⁺



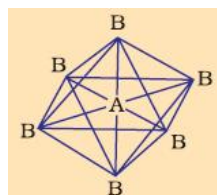
4) AB_5 type

Here there are 5 VSEPs. To reduce the repulsion, they are arranged at the five corners of a trigonal bipyramid with bond angles 120° and 90° . Eg. PCl_5



5) AB_6 type

Here there are 6 VSEPs. To reduce the repulsion, they are arranged at the six corners of an octahedron with bond angles 90° . Eg.: SF_6



II) Molecules containing both bond pairs and lone pairs

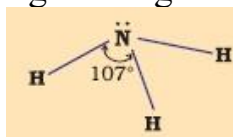
The presence of lone pairs of electron causes distortion in the shape of the molecules.

Type of molecule	Total no. of VSEPs	No. of BP	No. of LP	Shape	Example
AB_2E	3	2	1	Bent	SO_2, O_3
AB_3E	4	3	1	Trigonal Pyramid	NH_3
AB_2E_2	4	2	2	Bent	H_2O
AB_4E	5	4	1	See-saw	SF_4
AB_3E_2	5	3	2	T-Shape	ClF_3
AB_5E	6	5	1	Square Pyramid	BrF_5
AB_4E_2	6	4	2	Square Planar	XeF_4

Shapes of ammonia and water molecules by VSEPR theory

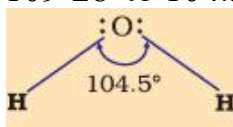
1. NH_3

In ammonia, the central atom N has 5 valence electrons ($7\text{N} - 2,5$). Among these electrons, three are used for the formation of bonds with hydrogen atoms and the remaining 2 electrons stay as lone pairs. So, there are 4 VSEPs. Hence the expected shape of the molecule is tetrahedral. But due to the presence of lone pairs, the shape is distorted to triangular pyramidal and the bond angle changes from $109^\circ 28'$ to 107° .



2. H_2O

In water, the central atom O has 6 valence electrons ($8\text{O} - 2,6$). Two of them are used for the formation of bonds with hydrogen atoms and the remaining 4 electrons stay as lone pairs. So, there are 4 VSEPs. Hence the expected shape of the molecule is tetrahedral. But due to the presence of 2 lone pairs, the shape is distorted bent or angular or inverted v shape and the bond angle changes from $109^\circ 28'$ to 104.5° .



Orbital overlap concept

Orbital overlapping is the process of partial interpenetration of atomic orbitals. The important characteristics of orbital overlapping are:

1. A covalent bond is formed by the overlapping of half-filled atomic orbitals present in the valence shell of atoms.
2. The overlapping orbitals should contain electron with opposite spin.
3. As a result of overlapping, the electrons get paired and a stable covalent bond is formed.
4. The strength of a covalent bond depends on the extent of overlapping. The greater the extent of overlapping, the stronger will be the covalent bond formed.

Types of overlapping

1. Axial overlapping:

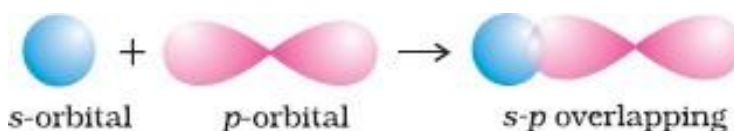
If the overlapping of atomic orbitals take place *along inter*

nuclear axis, it is called axial overlapping or end-to-end overlapping. A bond formed by axial overlapping is called **sigma (σ) bond**. The electrons present in sigma bond are called sigma electrons. All single bonds are sigma bonds.

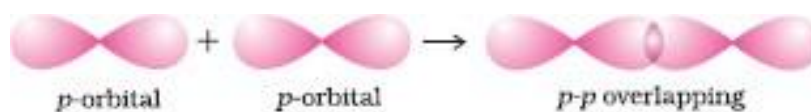
- i) s-s overlapping: The overlapping of two half-filled s-orbitals take place along the inter nuclear axis.



- ii) s-p overlapping: It occurs with the overlapping of one half-filled s-orbital and one half-filled p-orbital.

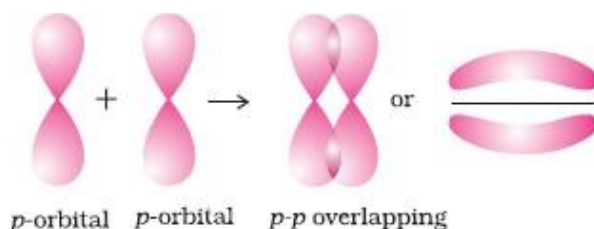


- i) p-p overlapping: The two half-filled p-orbitals of two atoms overlap.



2. Lateral overlapping:

The overlapping take place perpendicular to the inter nuclear axis. The bond formed as a result of lateral overlapping is called pi (π) bond. The electrons in pi bond are called π electrons.



A π bond is always present along with σ bonds. A double bond contains one σ bond and one π bond. A triple bond contains one sigma bond and two pi bonds. A sigma bond is stronger than a pi bond. This is because the extent of overlapping is greater in a sigma bond.

Hybridisation

It is the process of inter mixing atomic orbitals having slightly different energies to form new orbitals having equivalent energy and identical shape. The new orbitals formed are called hybrid orbitals.

Characteristics of hybridisation

1. The number of hybrid orbitals formed is equal to the number of atomic orbitals undergo hybridization.
2. The hybrid orbitals are always equivalent in energy and in identical shape.
3. The hybrid orbitals are more effective in forming stable bonds than the pure atomic orbitals.
4. The hybrid orbitals are directed to some fixed positions in space. So, the type of hybridization gives the shape of the molecule.

Important conditions of hybridisation

- a) The orbitals present in the valence shell of the atom are hybridized.
- b) The orbitals undergoing hybridization should have almost equal energy.
- c) Promotion of electrons is not an essential condition before hybridisation.
- d) Completely filled orbitals of valence shell can also take part in hybridisation.

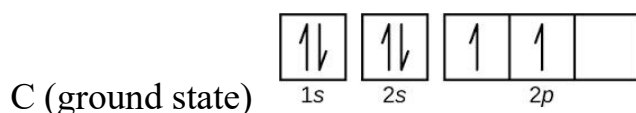
Types of hybridisation

1. sp^3 hybridisation

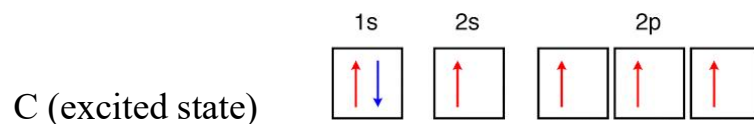
It is the process of inter mixing of one s-orbital and three p-orbitals to form four new orbitals having equivalent energy and shape. The 4 new orbitals formed are called sp^3 hybrid orbitals. They are directed to the four corners of a regular tetrahedron with bond angle $109^\circ 28'$. Each sp^3 hybrid orbitals has 25% s-character and 75% p-character.

e.g. i) **Formation of methane (CH_4)**

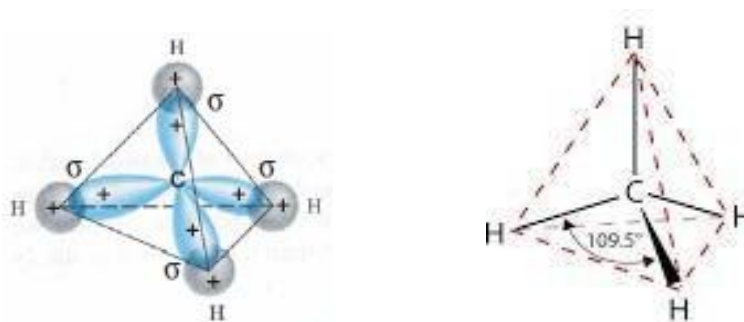
In CH_4 , the central atom C has the electronic configuration
 $6C - 1s^2 2s^2 2p^2$



In excited states, the electrons of 2s orbital is promoted to 2p orbital.

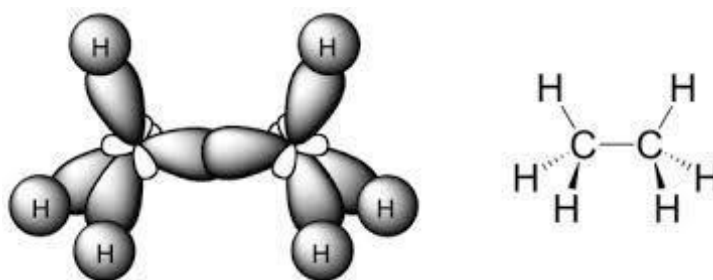


The one s-orbital and three p-orbitals undergo sp^3 hybridisation. These sp^3 hybrid orbitals are directed to the four corners of a regular tetrahedron with bond angle $109^\circ 28'$. Each of these sp^3 hybrid orbitals overlap with 1s orbital of H to form four C-H σ bonds.



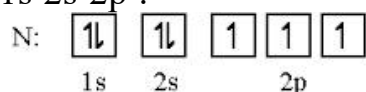
ii) Formation of ethane (C₂H₆)

In ethane, each C atom undergoes sp^3 hybridisation. Out of the 4 sp^3 hybrid orbitals, one of each C atom overlaps axially to form a C-C σ bond. The remaining 3 sp^3 hybrid orbitals of each C atom overlap with 1s orbital of H atom to form 6 C-H σ bonds.



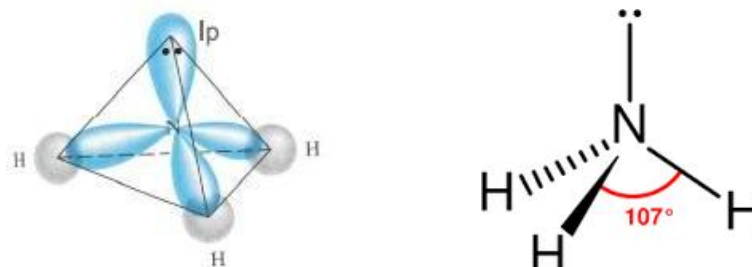
ii) Formation of Ammonia (NH₃) molecule

In NH₃, the central atom N has the electronic configuration $1s^2 2s^2 2p^3$.



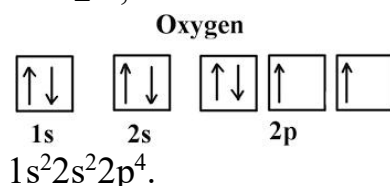
The one s-orbital and three p-orbitals of N undergo sp^3 hybridisation to form 4 sp^3 hybrid orbitals. One of this sp^3 hybrid orbitals is occupied by a lone pair and the other three sp^3 hybrid orbitals overlap with 1s orbital of

hydrogen to form 3 N-H bonds. Due to the greater repulsion between lone pair and bond pairs, the shape is distorted to **pyramidal** and the bond angle becomes **107°**.



ii) **Formation of water (H_2O) molecule**

In H_2O , the central atom O has the electronic configuration



The one s-orbital and three p-orbitals of O undergo sp^3 hybridisation to form 4 sp^3 hybrid orbitals. Two of these sp^3 hybrid orbitals are occupied by lone pairs and the other two sp^3 hybrid orbitals overlap with 1s orbital of hydrogen to form 2 O-H bonds. Due to the greater repulsion between lone pairs, the shape is distorted to angular shape or bent structure or inverted 'v' shape and the bond angle becomes 104.5°.



2. sp^2 hybridisation

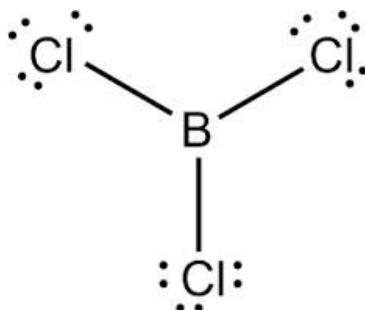
It is the process of inter mixing of one s-orbital and two p-orbitals to form three new orbitals having equivalent energy and shape. The 3 new orbitals formed are called sp^2 hybrid orbitals. They are directed to the three

corners of an equilateral triangle. So, the shape of the molecule is planar triangular or trigonal planar with bond angle 120° . Each sp^2 hybrid orbital has 33% s-character and 66% p-character.

e.g. i) **Formation of BCl_3**

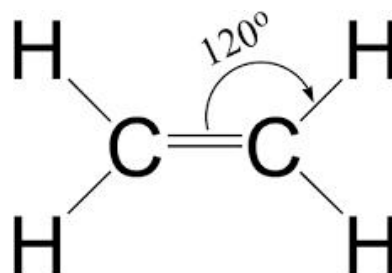
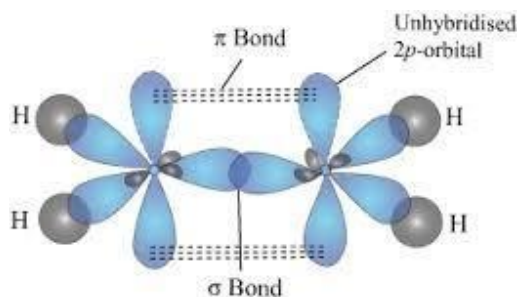
The central atom B has the electronic configuration $1s^2 2s^2 2p^1$. In the excited state, one of the 2s electrons is promoted to vacant 2p orbital. So, the configuration becomes $2s^1 2p^2$.

The one s-orbital and two p-orbitals undergo hybridisation. The 3 hybrid orbitals formed overlap with 2p orbitals of Cl to form 3 B-Cl σ bonds. Since the hybridisation is sp^2 , the shape of the molecule is planar triangular with bond angle 120° .



ii) **Formation of ethene or ethylene (C_2H_4)**

In ethene, each C atom undergoes sp^2 hybridisation. Out of the 3 sp^2 hybrid orbitals, one of each C overlaps axially to form a C-C σ bond. The remaining two sp^2 hybrid orbitals of each C overlap with the 1s orbital of H to form 4 C-H σ bonds. The each C atom has one unhybridized p-orbital, which overlaps laterally to form a π bond. Thus, there are 5 σ bonds and one π bond in ethene.



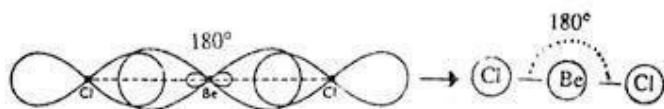
3. sp hybridisation:

It is the process of inter mixing of one s-orbital and one p-orbital to form two new orbitals having equivalent energy and shape. The 2 new orbitals formed are called sp hybrid orbitals. The shape is linear with bond angle 180° . Each sp hybrid orbitals has 50% s-character and 50% p-character.

e.g. i) *Formation of BeCl_2*

in BeCl_2 , the central atom Be has the electronic configuration $1s^2 2s^2$. In the excited state, one of the 2s electrons is promoted to 2p level. So, the configuration becomes $1s^2 2s^1 2p^1$.

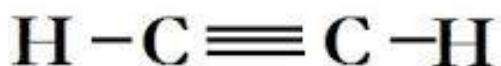
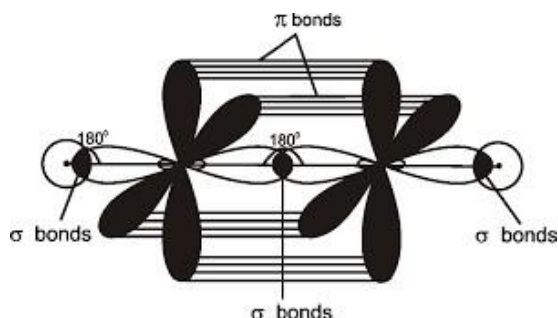
The one s-orbital and one p-orbital undergo sp hybridisation to form 2 new sp hybrid orbitals. Each of these hybrid orbitals overlaps with the 2p orbitals of Cl to form 2 Be-Cl bonds. The shape of the molecule is linear with bond angle 180° .



ii) *Formation of ethyne or acetylene (C_2H_2)*

In acetylene, each C atom undergoes sp hybridisation. Out of the 2 sp hybrid orbitals, one of each C overlaps axially to form a C-C σ bond. The remaining two sp hybrid orbitals of each C overlap with the 1s orbital of H to form 2 C-H σ bonds.

The each C atom has 2 unhybridized p-orbitals, which overlap laterally to form 2 π bonds. Thus, the molecule has linear shape with bond angle 180° . Here there are 3 σ bonds and 2 π bonds in ethyne.

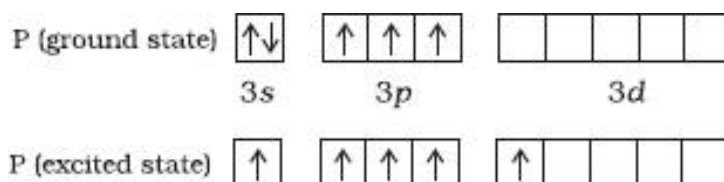


4. sp^3d hybridisation

It is the process of inter mixing of one s-orbital, three p-orbitals and one d-orbital to form five new orbitals having equivalent energy and shape. The 5 new orbitals formed are called sp^3d hybrid orbitals. These are directed to the five corners of a regular trigonal bipyramid with bond angles 120° and 90° .

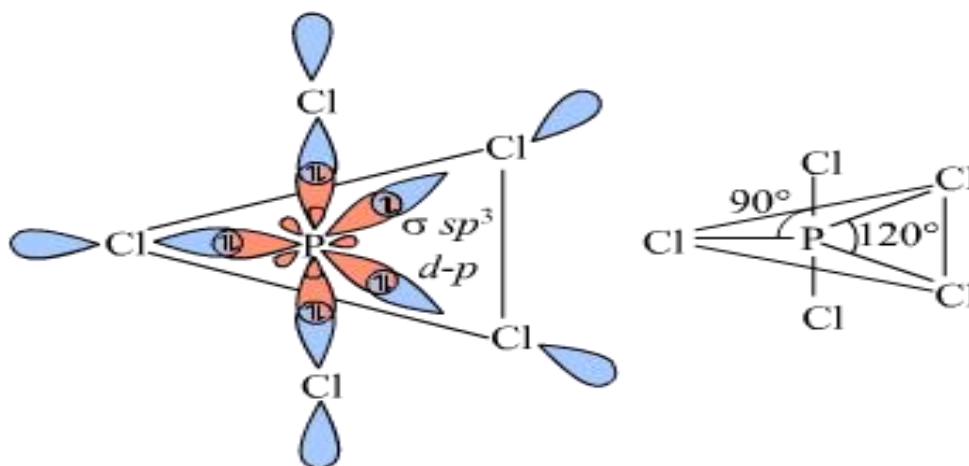
E.g. *Formation of PCl_5*

In PCl_5 , the central atom P has the electronic configuration $15P - [Ne] 3s^2 3p^3 3d^0$. To satisfy the Penta valency of P, one of the 3s electrons is promoted to 3d level.



Now, one s-orbital, three p-orbitals and one d-orbital undergo sp^3d hybridisation. These 5 sp^3d hybrid orbitals are directed to the five corners of a regular trigonal bipyramid with bond angles 120° and 90° .

In PCl_5 , three P-Cl bonds lie in one plane, at an angle of 120° . These three bonds are called equatorial bonds. The other two P-Cl bonds lie one above and one below this plane. They are called axial bonds. The axial bond pairs suffer more repulsion from the equatorial bond pairs. So, the axial bond length is greater than the equatorial bond length. So PCl_5 is highly unstable and is very reactive.



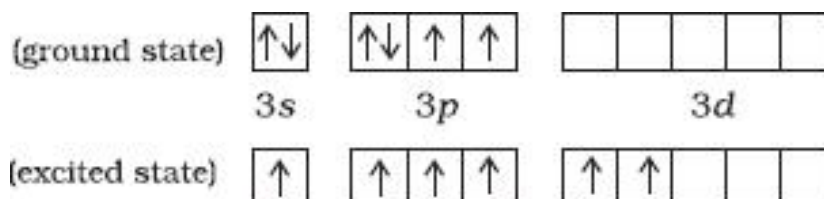
Trigonal bipyramidal structure of PCl_5

5. sp^3d^2 hybridisation

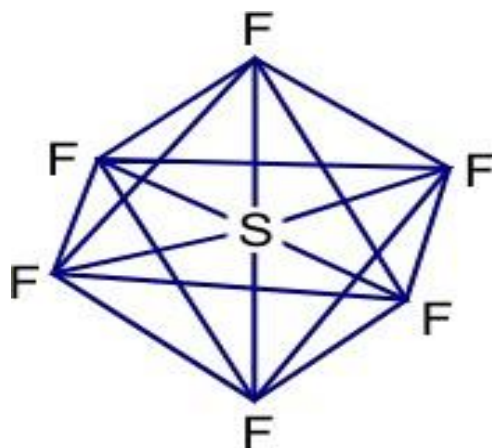
It is the process of inter mixing of one s-orbital, three p-orbitals and two d-orbitals to form six new orbitals having equivalent energy and shape. The 6 new orbitals formed are called sp^3d^2 hybrid orbitals. These are directed to the six corners of a regular octahedron with bond angle 90° .

e.g. *Formation of SF_6*

In SF_6 the central sulphur atom has the ground state outer electronic configuration $3s^23p^4$. In the excited state one electron each from 3s and 3p orbitals are promoted to 3d level.



The one s-orbital, three p-orbitals and two d-orbitals undergo sp^3d^2 hybridisation. These hybrid orbitals overlap with p-orbitals of fluorine atoms to form 6 S–F sigma bonds. Thus, SF_6 molecule has a regular octahedral geometry with bond angle 90° .



Molecular Orbital Theory

This theory was developed by F.Hund and R.S Mulliken. The important postulates of this theory are:

- 1) In molecules, the electrons are present in some special type of orbitals called molecular orbitals (M.Os).
- 2) The atomic orbitals (A.Os) of comparable energy and proper symmetry combine to form molecular orbitals.
- 3) Atomic orbitals are monocentric, while molecular orbitals are polycentric. The electrons present in atomic orbitals are attracted by only one nucleus. While the electrons present in molecular orbitals are attracted by more than one nucleus.
- 4) The number of molecular orbitals formed = the number of atomic orbitals combined. i.e. if 2 atomic orbitals combined, 2 molecular orbitals are formed. One is called bonding molecular orbital (BMO) and the other is called anti-bonding molecular orbitals (AMO)
- 5) The BMO has lower energy and greater stability than the corresponding AMO.
- 6) The molecular orbitals give the electron probability distribution around a group of nuclei.
- 7) The molecular orbitals are filled according to 3 rules – Aufbau principle, Pauli's exclusion principle and Hund's rule.

Formation of molecular orbitals – Linear Combination of Atomic Orbitals (LCAO) method

According to this theory, the combinations of atomic orbitals take place by addition and subtraction of wave functions of atomic orbitals. The M. O formed by the addition of A.Os is called the bonding molecular orbital (BMO) and by the subtraction of A.Os is called the anti-bonding molecular orbitals (AMO).

The electron density in a BMO is located between the nuclei of the bonded atoms. So, the repulsion between the nuclei is very low. Therefore, a BMO always possess lower energy than the combining

A.Os. While in the case of an AMO, most of the electron density is located away from the space between the nuclei. There is a nodal plane between the nuclei and hence the repulsion between the nuclei is high. So, an AMO possess higher energy than the combining A.Os. AMO is denoted by using an asteric (*) mark.

Conditions for the combination of atomic orbitals

The combination of A.Os to form M.Os takes place only if the following conditions are satisfied:

1. The combining A.Os must have the same or nearly the same energy.
2. The combining A.Os must have the same symmetry about the molecular axis.
3. The combining A.Os must overlap to the maximum extent.

Types of molecular orbitals

M.Os of diatomic molecules are designated as σ (sigma), π (Pi), δ (delta) etc. the sigma M.Os are symmetrical

about the bond axis, while the pi M.Os are not symmetrical.

Linear combination of two 1s atomic orbitals produces two M.Os – a BMO σ_{1s} and an AMO σ^*_{1s} .

Similarly linear combination of two 2s atomic orbitals produces two M.Os – σ_{2s} and σ^*_{2s} . If z-axis is taken as the inter nuclear axis, linear combination of two 2pz orbitals produces two sigma M.Os σ_{2pz} and σ^*_{2pz} .

While the combination of 2px and 2py orbitals produce M.Os which are not symmetrical about the bond axis. The two 2px orbitals produces 2 sigma M.Os – π_{2px} and π^*_{2px} and two 2py orbitals produce 2 M.Os – π_{2py} and π^*_{2py} .

Energies of various M.Os

The various M.Os are filled in the increasing order of their energies (Aufbau Principle).

The increasing order of energy for H₂ to N₂ is:

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

For O₂, F₂ and Ne₂, the order is:

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

Bond Order

It is defined as *the half of the difference between the number of bonding electrons (N_b) and the number of anti-bonding electrons (N_a)*.

$$\text{Bond order (B.O)} = \frac{1}{2} [N_b - N_a]$$

A molecule is stable only if the bond order is positive. (i.e. $N_b > N_a$). a negative bond order (i.e. $N_b < N_a$ or $N_b = N_a$) means an unstable molecule.

For a single bond, B.O = 1, for a double bond B.O = 2 and so on. Bond order gives an approximate measure of the bond length. In general, *as the bond order increases, bond length decreases and bond enthalpy increases.*

Molecular orbital configuration and Bond order of some Homonuclear diatomic molecules

Molecule	M.O configuration	Total no. of electrons	No. of Bonding Electrons (N_b)	No. of Anti-bonding electrons (N_a)	Bond Order $\text{B.O} = \frac{1}{2} [N_b - N_a]$
H ₂	$\sigma 1s^2$	2	2	0	$= \frac{1}{2} [2 - 0] = \frac{1}{2} \times 2 = 1$
He ₂	$\sigma 1s^2 \sigma^* 1s^2$	4	2	2	$= \frac{1}{2} [2 - 2] = \frac{1}{2} \times 0 = 0$
Li ₂	$\sigma 1s^2 \sigma^* 1s^2 \sigma 2s^2$	6	4	2	$= \frac{1}{2} [4 - 2] = \frac{1}{2} \times 2 = 1$
Be ₂	$\sigma 1s^2 \sigma^* 1s^2 \sigma 2s^2 \sigma^* 2s^2$	8	4	4	$= \frac{1}{2} [4 - 4] = \frac{1}{2} \times 0 = 0$
B ₂	$\sigma 1s^2 \sigma^* 1s^2 \sigma 2s^2 \sigma^* 2s^2$ $\pi 2p_x^1 \pi 2p_y^1$	1 0	6	4	$= \frac{1}{2} [6 - 4] = \frac{1}{2} \times 2 = 1$
C ₂	$\sigma 1s^2 \sigma^* 1s^2 \sigma 2s^2 \sigma^* 2s^2$ $\pi 2p_x^2 \pi 2p_y^2$	1 2	8	4	$= \frac{1}{2} [8 - 4] = \frac{1}{2} \times 4 = 2$
N ₂	$\sigma 1s^2 \sigma^* 1s^2 \sigma 2s^2 \sigma^* 2s^2$ $\pi 2p_x^2 \pi 2p_y^2$ $\sigma 2p_z^1$	1 4	10	4	$= \frac{1}{2} [10 - 4] = \frac{1}{2} \times 6 = 3$
O ₂	$\sigma 1s^2 \sigma^* 1s^2 \sigma 2s^2 \sigma^* 2s^2$ $\sigma 2p_z^2 \pi 2p_x^2 \pi 2p_y^2$ $\pi^* 2p_x^1 \pi^* 2p_y^1$	1 6	10	6	$= \frac{1}{2} [10 - 6] = \frac{1}{2} \times 4 = 2$
F ₂	$\sigma 1s^2 \sigma^* 1s^2 \sigma 2s^2 \sigma^* 2s^2$ $\sigma 2p_z^2 \pi 2p_x^2 \pi 2p_y^2$ $\pi^* 2p_x^2 \pi^* 2p_y^2$	1 8	10	8	$= \frac{1}{2} [10 - 8] = \frac{1}{2} \times 2 = 1$
Ne ₂	$\sigma 1s^2 \sigma^* 1s^2 \sigma 2s^2 \sigma^* 2s^2$ $\sigma 2p_z^2 \pi 2p_x^2 \pi 2p_y^2$ $\pi^* 2p_x^2 \pi^* 2p_y^2 \sigma^* 2p_z^2$	2 0	10	10	$= \frac{1}{2} [10 - 10] = \frac{1}{2} \times 0 = 0$

He₂, Be₂ and Ne₂ molecules do not exist, since their Bond orders are zero. H₂, Li₂, B₂ and F₂ molecules contain a single bond, since their bond order = 1, C₂ and O₂ molecules contain a double bond, since their B.O = 2 and for N₂, there is a triple bond since its bond order = 3.

Magnetic nature

If all the M.Os in a molecule are doubly occupied, the substance is diamagnetic. The substance is repelled by an external magnetic field. If one or more M.Os are singly occupied, it is paramagnetic. It is attracted by an external magnetic field. Eg. O₂ molecule.

Molecular orbital Diagram

The representation of various M.Os in the increasing order of energy is called M.O diagram.

Bonding in Some Homonuclear Diatomic Molecules

1. Hydrogen (H₂) Molecule

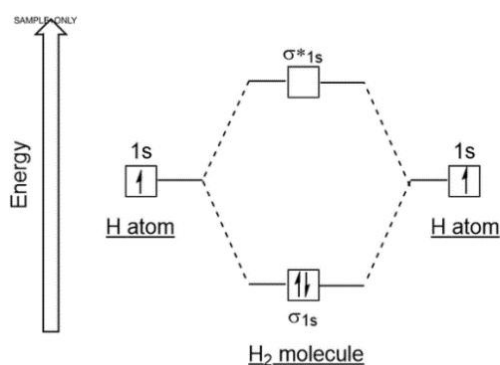
H₂ molecule is formed by the combination of two Hydrogen atoms.



Total no. of electrons in H₂ molecule = 2

M.O configuration is $\sigma 1s^2$

The M.O diagram for H₂ molecule is



2. Carbon (C₂) Molecule

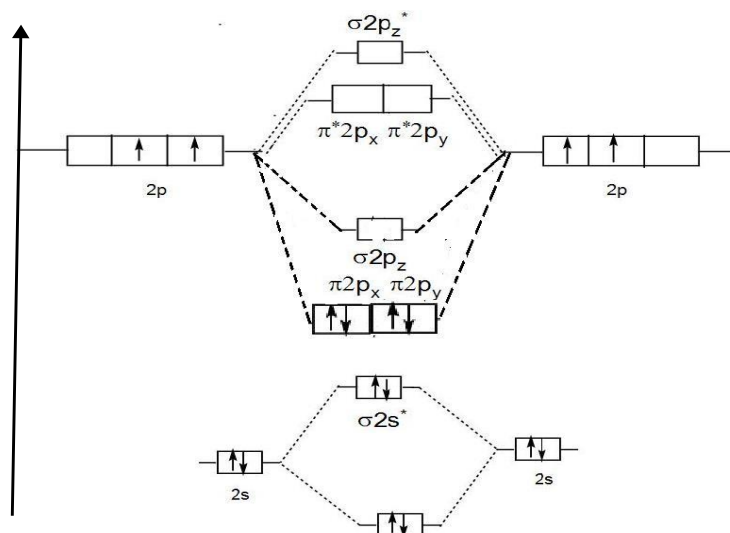
C₂ molecule is formed by the combination of two Carbon atoms.



Total no. of electrons in C₂ molecule = 12

M.O configuration is $\sigma 1s^2 \sigma^* 1s^2 \sigma 2s^2 \sigma^* 2s^2 \pi 2p^2 \pi 2p^2$

Its M.O diagram is:



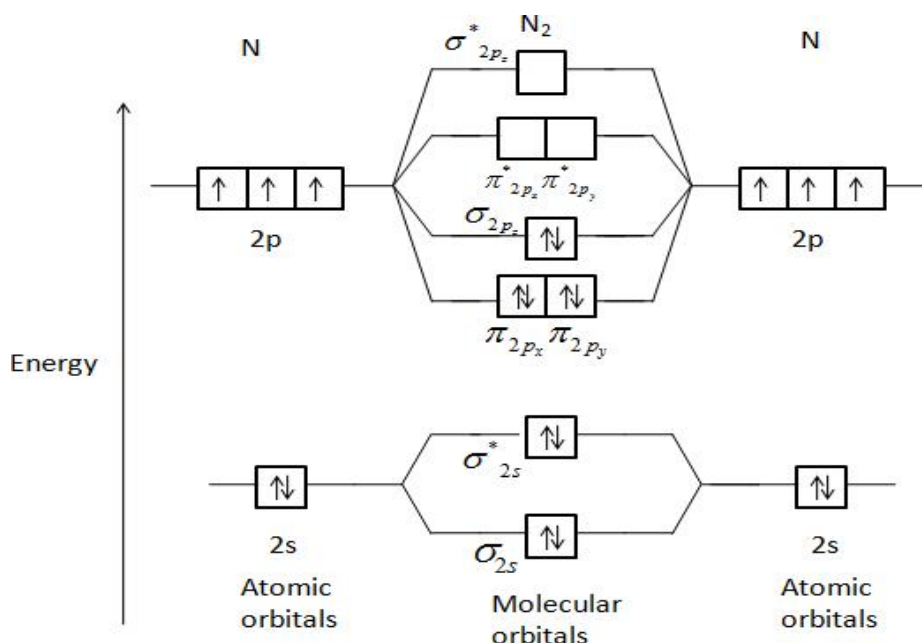
3. Nitrogen (N₂) Molecule

N₂ molecule is formed by the combination of two Nitrogen atoms.

Total no. of electrons in N₂ molecule = 14

M.O configuration is = $\sigma 1s^2 \sigma^* 1s^2 \sigma 2s^2 \sigma^* 2s^2 \pi 2p_x^2 \pi 2p_y^2 \sigma 2p_z^2$

Due to the absence of unpaired electrons, N₂ molecule is diamagnetic.

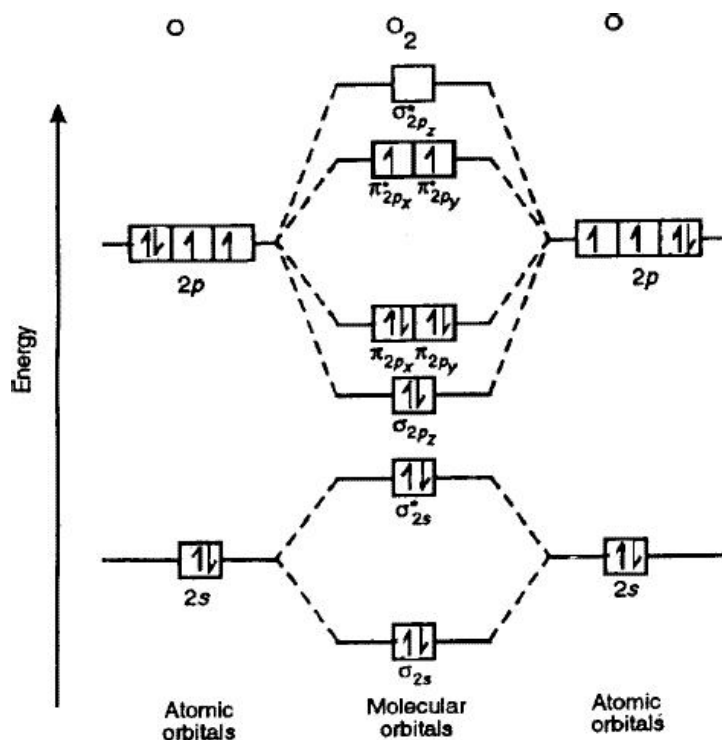


4. Oxygen (O₂) molecule

O₂ molecule is formed by the combination of two Oxygen atoms.

Total no. of electrons in O₂ molecule = 16

M.O configuration is = $\sigma 1s^2 \sigma^* 1s^2 \sigma 2s^2 \sigma^* 2s^2 \sigma 2p_z^2 \pi 2p_x^2 \pi 2p_y^2 \pi^* 2p_x^1 \pi^* 2p_y^1$ Due to the presence of unpaired electrons, O₂ molecule is paramagnetic



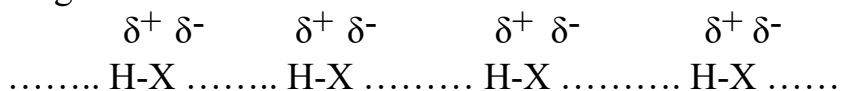
Hydrogen Bonding

The weak attractive force between Hydrogen atom of one molecule and electronegative atom (like F, O or N) of the same or different molecule is termed as Hydrogen bond. It is weaker than a covalent bond but stronger than van der Waal's force. It is represented by dotted line.

Cause of Hydrogen bonding:

When hydrogen is bonded to a strongly electronegative atom X, the shared electron pair is shifted more towards X. So, Hydrogen atom gets a slight positive charge (δ^+) and the electronegative atom gets a slight negative charge (δ^-). This results in the formation of a polar molecule.

The electrostatic force of attraction between these polar molecules is termed as H-bonding.



Types of Hydrogen bonds

There are two types of H bonds- inter molecular hydrogen bonding and intra molecular hydrogen bonding.

1) Inter molecular Hydrogen bonding:

It is the hydrogen bond formed by H atom of one molecule and the electronegative atom of another molecule.

Eg. H_2O , H-F, NH_3

Inter molecular H bonding influences the physical properties of the compounds. The water (H_2O) is a liquid with high boiling point but hydrogen sulphide (H_2S) is a gas. This is because in water inter molecular H bonding is possible which is not possible in H_2S .

2. Intra molecular Hydrogen bonding: It is the hydrogen bond formed between H atom and the electronegative atom of the same molecule.

e.g. Hydrogen bonding in ortho-nitrophenol

