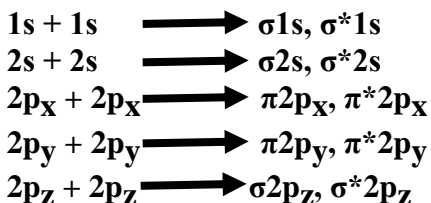


MOLECULAR ORBITAL THEORY: This theory was given by F.Hund & R.S.Mulliken in 1932. The main points of this theory are as follows:

1. In molecules atomic orbitals lose their identity and the electrons are present in new orbitals. These new orbitals are called molecular orbitals.
2. Molecular orbitals are formed by the LCAO (linear combination of atomic orbitals) of nearly same energies.



3. The numbers of molecular orbitals formed are equal to the number of atomic orbitals combined.
4. There are two types of molecular orbitals:

A. Bonding molecular orbitals (BMO's):

- These molecular orbitals are formed by the addition of wave functions of two atomic orbitals.

$$\Psi_{\text{BMO}} = \Psi_A + \Psi_B$$

- Bonding molecular orbitals have lower energy than the pure atomic orbitals.
- Bonding molecular orbitals have high electron density than pure atomic orbitals
- $\Psi_A^2 + \Psi_B^2 < (\Psi_A + \Psi_B)^2 = \Psi_A^2 + \Psi_B^2 + 2\Psi_A\Psi_B$
- Bonding molecular orbitals provide stability to the molecules and help in bond formation.
- Bonding molecular orbitals are represented by σ & π

B. Antibonding molecular orbitals (ABMO's):

- Antibonding molecular orbitals are formed by the subtraction of wave functions of two atomic orbitals.

$$\Psi_{\text{ABMO}} = \Psi_A - \Psi_B$$

- Antibonding molecular orbitals have higher energy than the pure atomic orbitals.
- Antibonding molecular orbitals have low electron density than pure atomic orbitals
- $\Psi_A^2 + \Psi_B^2 > (\Psi_A - \Psi_B)^2 = \Psi_A^2 + \Psi_B^2 - 2\Psi_A\Psi_B$
- Antibonding molecular orbitals do not provide stability to the molecule.
- Antibonding molecular orbitals are represented by σ^* & π^*

5. Molecular orbitals are represented by a set of quantum numbers.
6. Electrons are entered in molecular orbitals increasing order of their energy. The increasing order of energy of molecular orbitals are as follows:

A. For molecules having total electrons ≤ 14

$$\sigma 1s < \sigma^* 1s < \sigma 2s < \sigma^* 2s < (\pi 2p_x = \pi 2p_y) < \sigma 2p_z < (\pi^* 2p_x = \pi^* 2p_y) < \sigma^* 2p_z$$

B. For molecules having total electrons ≥ 15

$$\sigma 1s < \sigma^* 1s < \sigma 2s < \sigma^* 2s < \sigma 2p_z < (\pi 2p_x = \pi 2p_y) < (\pi^* 2p_x = \pi^* 2p_y) < \sigma^* 2p_z$$

7. **Bond Order:** The total number of covalent bonds present between two atoms is called bond order. It can be calculated with the help of MOT

$$\text{Bond Order (BO)} = (N_b - N_a) / 2$$

Where N_b = number of electrons in bonding molecular orbitals.

N_a = number of electrons in antibonding molecular orbitals.

8. **Magnetic nature:** magnetic nature of a molecule or ion can be explained with the help of MOT.
Molecules having unpaired electrons in molecular orbitals are **paramagnetic** in nature.
Molecules does not have unpaired electrons in molecular orbitals are **diamagnetic** in nature.
9. For a stable molecule $N_b > N_a$
10. The maximum number of electrons present in a molecular orbital is two with opposite spin.

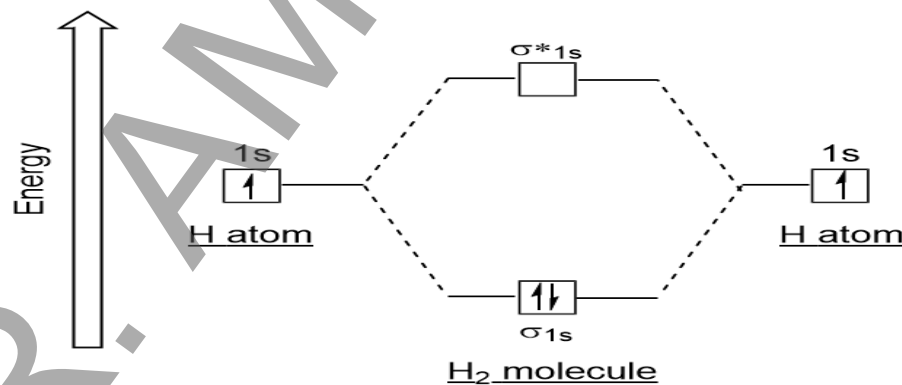
DIATOMIC MOLECULES: Those molecules which are formed by the combination of two atoms are called diatomic molecules.

There are two types of diatomic molecules.

1. **Homonuclear diatomic molecules:** Those molecules which are formed by the combination of two atoms of same element are called Homonuclear diatomic molecules.
For Example: $H_2, H_2^+, He_2, He_2^+, Li_2, Be_2, N_2, N_2^+, N_2^{++}, N_2^-, N_2^{--}, O_2, O_2^+, O_2^{++}, O_2^-, O_2^{--}, F_2, Ne_2$
2. **Heteronuclear diatomic molecules:** Those molecules which are formed by the combination of two atoms of different elements are called Heteronuclear diatomic molecules.
For Example: $CO, NO, HF, HCl, NO^+, NO^-$.

EXAMPLES OF HOMONUCLEAR DIATOMIC MOLECULES AND MOLECULAR IONS:

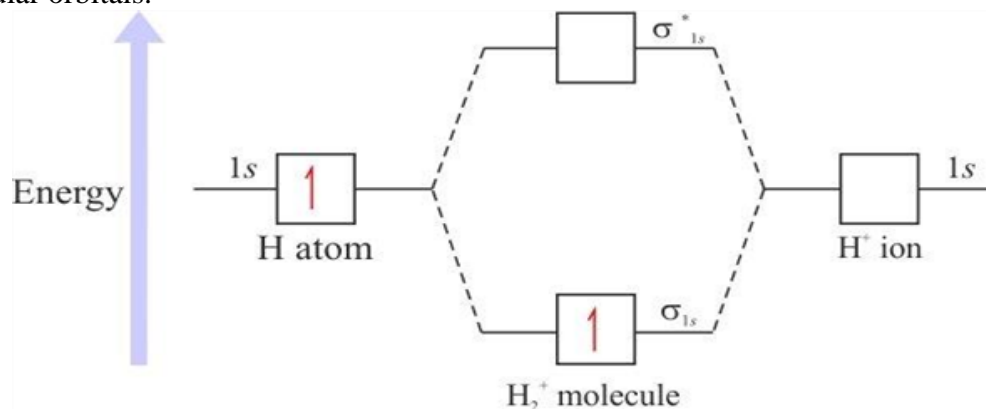
1. **H_2 Molecule:** It is formed by the combination of two hydrogen atoms.
H atom + H atom = H_2 molecule ($1s^1 + 1s^1$)
Total number of electrons in H_2 molecule = $1 + 1 = 2$
MOC: $\sigma 1s^2, \sigma^* 1s$
B.O. = $(N_b - N_a)/2 = (2 - 0)/2 = 1$ (**H – H**)
Magnetic Nature: It is diamagnetic in nature due to absence of unpaired electrons in molecular orbitals.



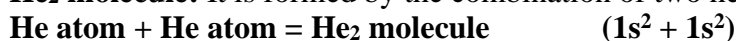
2. **H_2^+ Molecular Ion:** It is formed by the combination of H atom and H^+ ion.
H atom + H^+ ion = H_2^+ Molecular Ion ($1s^1 + 1s^0$)
Total number of electrons in H_2^+ Molecular Ion = $1 + 0 = 1$
MOC: $\sigma 1s^1, \sigma^* 1s$

$$\text{B.O.} = (\text{N}_b - \text{N}_a)/2 = (1-0)/2 = 0.5$$

Magnetic Nature: It is paramagnetic in nature due to presence of unpaired electrons in molecular orbitals.



3. **He₂ molecule:** It is formed by the combination of two helium atoms.



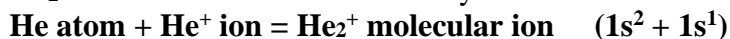
Total number of electrons in He₂ molecule = 2 + 2 = 4

MOC: $\sigma 1s^2, \sigma^* 1s^2$

$$\text{B.O.} = (\text{N}_b - \text{N}_a)/2 = (2-2)/2 = 0$$

Because B.O. is zero so He₂ molecule dose not exist.

4. **He₂⁺ molecular ion:** It is formed by the combination of He atom and He⁺ ion.

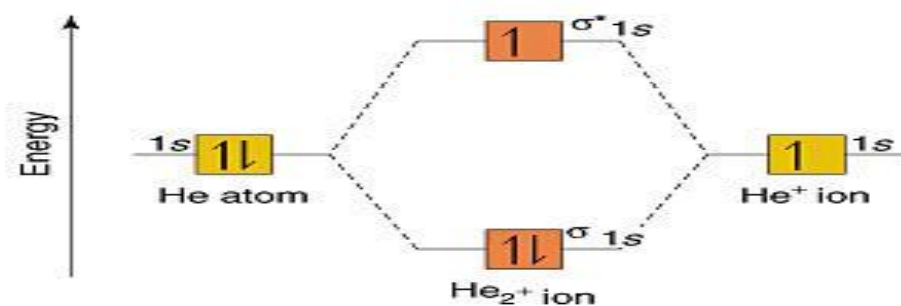


Total number of electrons in He₂⁺ molecular ion = 2 + 1 = 3

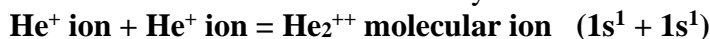
MOC: $\sigma 1s^2, \sigma^* 1s^1$

$$\text{B.O.} = (\text{N}_b - \text{N}_a)/2 = (2-1)/2 = 0.5$$

Magnetic Nature: It is paramagnetic in nature due to presence of unpaired electrons in molecular orbitals.



5. **He₂⁺⁺ molecular ion:** It is formed by the combination of two He⁺ ions.

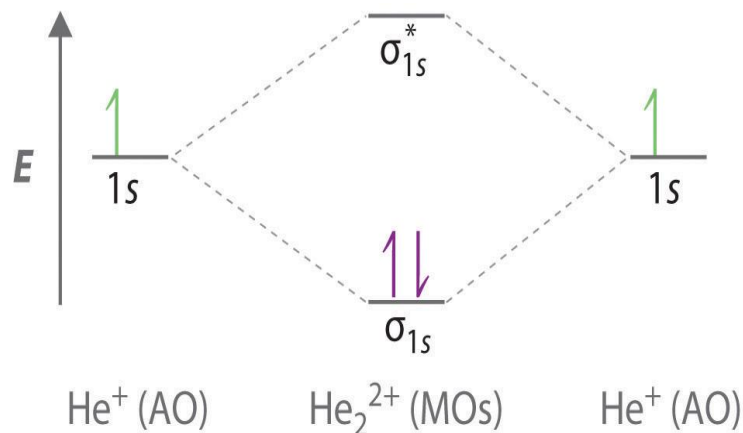


Total number of electrons in He₂⁺⁺ molecular ion = 1 + 1 = 2

MOC: $\sigma 1s^2, \sigma^* 1s$

$$\text{B.O.} = (\text{N}_b - \text{N}_a)/2 = (2-0)/2 = 1$$

Magnetic Nature: It is diamagnetic in nature due to absence of unpaired electrons in molecular orbitals.



6. **Li_2 molecule:** It is formed by the combination of two lithium atoms.

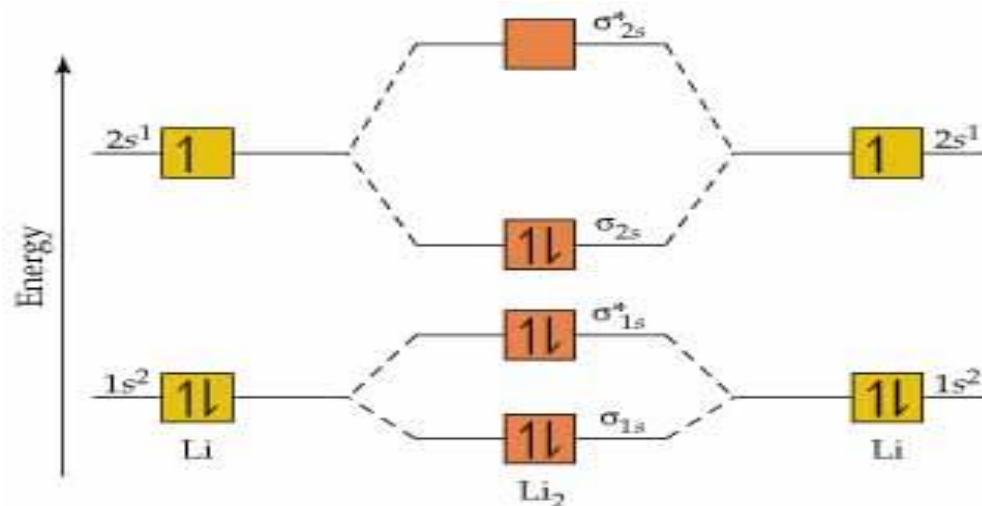
Li atom + Li atom = Li_2 molecule ($1s^2, 2s^1 + 1s^2, 2s^1$)

Total number of electrons in Li_2 molecule = $3 + 3 = 6$

MOC: $\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s$

B.O. = $(N_b - N_a)/2 = (4 - 2)/2 = 1$

Magnetic Nature: It is diamagnetic in nature due to absence of unpaired electrons in molecular orbitals.



7. **Be_2 molecule:** It is formed by the combination of two beryllium atoms.

Be atom + Be atom = Be_2 molecule ($1s^2, 2s^2 + 1s^2, 2s^2$)

Total number of electrons in Be_2 molecule = $4 + 4 = 8$

MOC: $\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2$

B.O. = $(N_b - N_a)/2 = (4 - 4)/2 = 0$

Because B.O. is zero so Be_2 molecule does not exist.

8. **N₂ Molecule:** It is formed by the combination of two Nitrogen atoms.

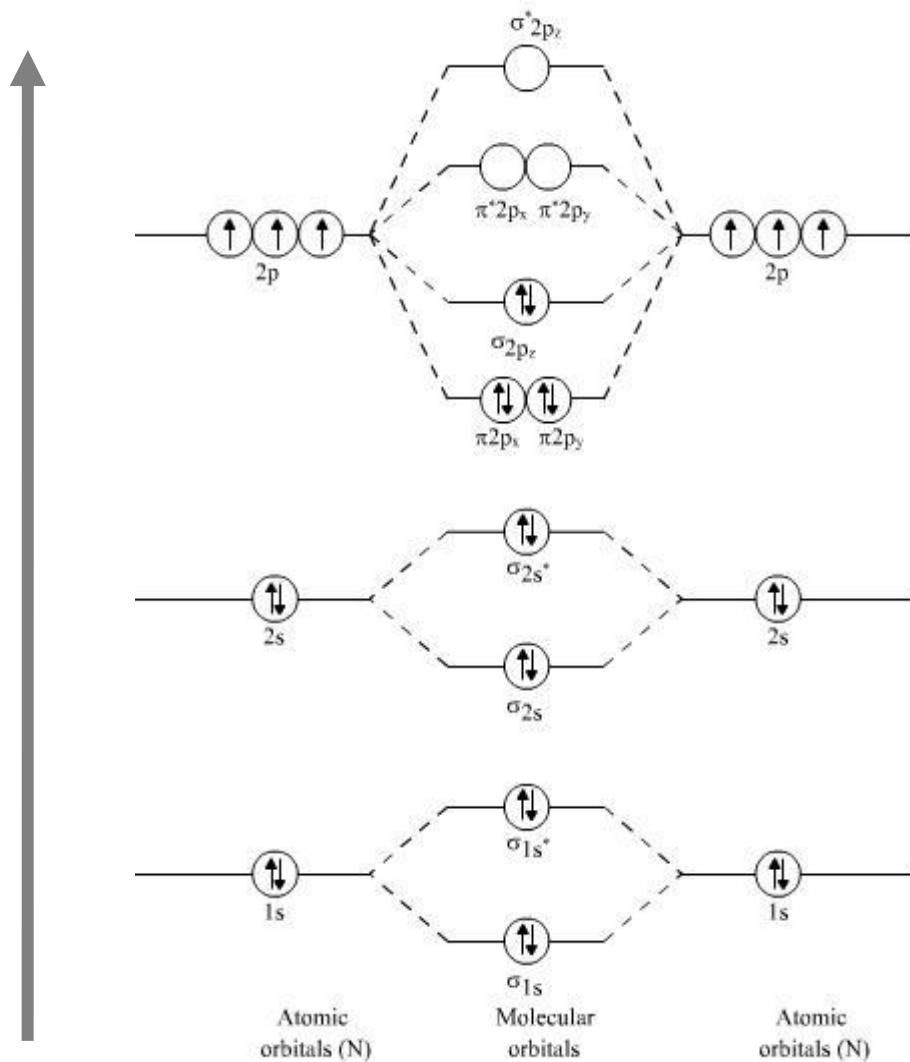


Total number of electrons in N₂ molecule = 7 + 7 = 14

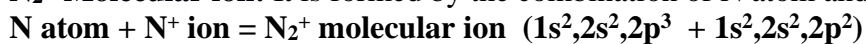
MOC: $\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \pi 2p_x^2 = \pi 2p_y^2, \sigma 2p_z^2, \pi^* 2p_x = \pi^* 2p_y, \sigma^* 2p_z$

B.O. = $(N_b - N_a)/2 = (10 - 4)/2 = 3$

Magnetic Nature: It is diamagnetic in nature due to absence of unpaired electrons in molecular orbitals.



9. **N₂⁺ Molecular ion:** It is formed by the combination of N atom and N⁺ ion.

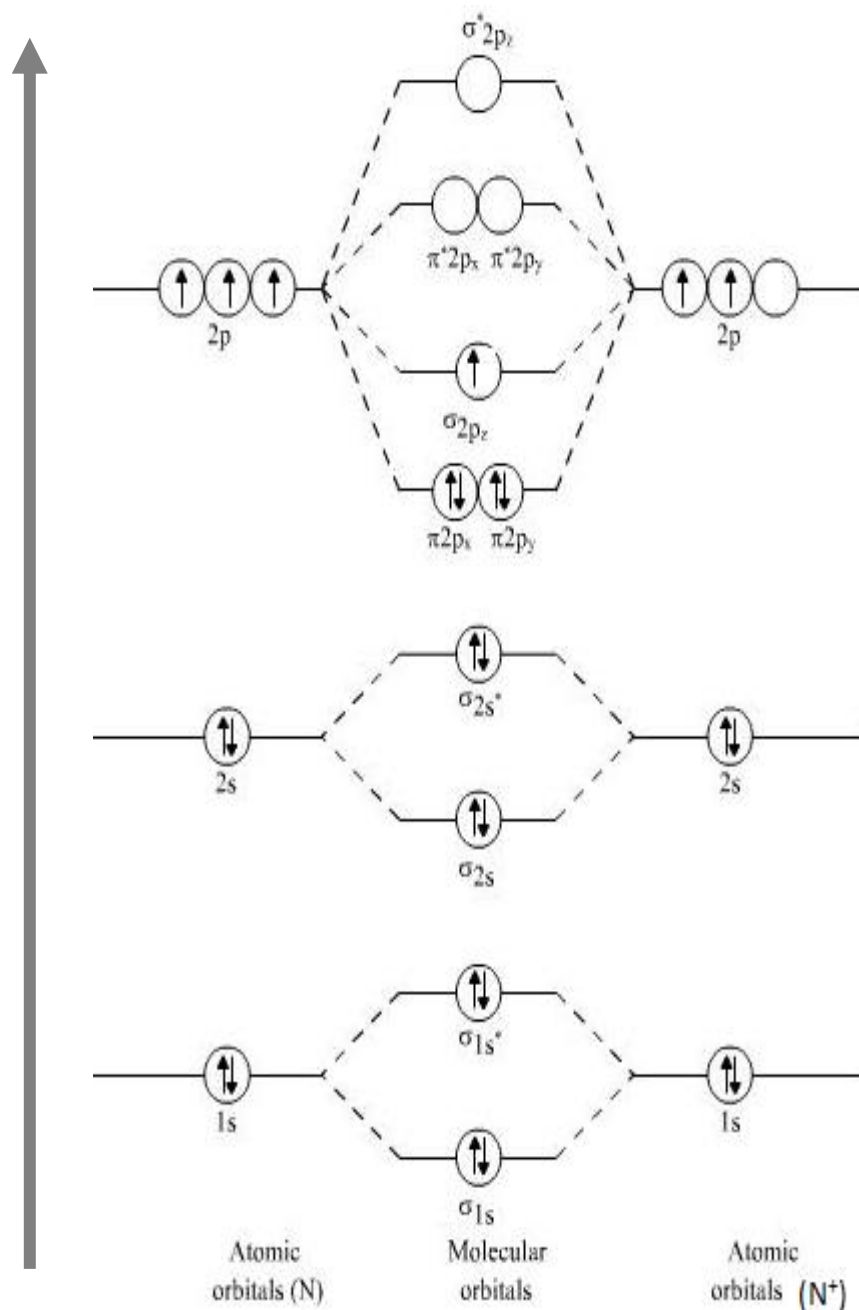


Total number of electrons in N₂⁺ molecular ion = 7 + 6 = 13

MOC: $\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \pi 2p_x^2 = \pi 2p_y^2, \sigma 2p_z^1, \pi^* 2p_x = \pi^* 2p_y, \sigma^* 2p_z$

B.O. = $(N_b - N_a)/2 = (9 - 4)/2 = 2.5$

Magnetic Nature: It is paramagnetic in nature due to presence of unpaired electrons in molecular orbitals.



10. N₂⁺⁺ Molecular ion: It is formed by the combination of two N⁺ ions.

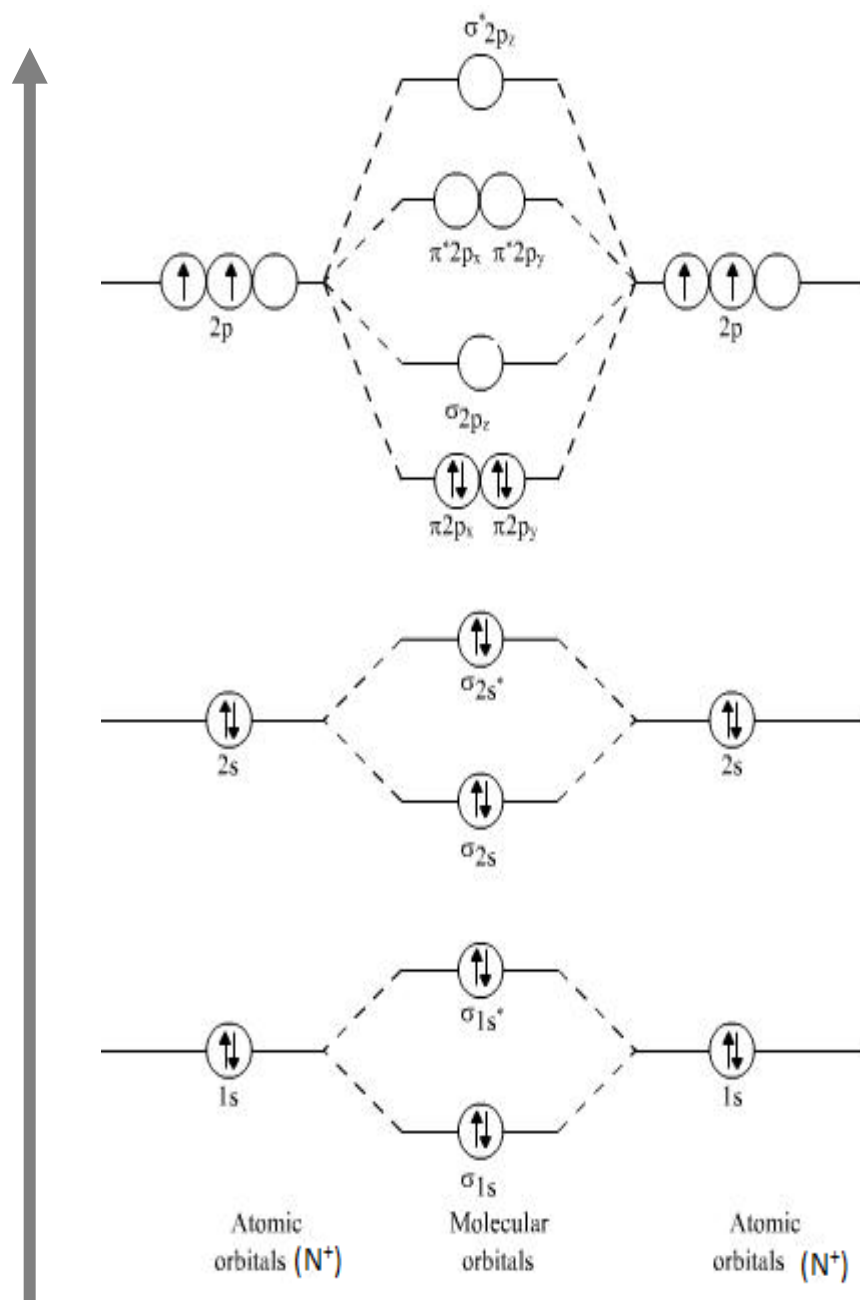
N⁺ ion + N⁺ ion = N₂⁺⁺ molecular ion (1s², 2s², 2p² + 1s², 2s², 2p²)

Total number of electrons in N₂⁺⁺ molecular ion = 6 + 6 = 12

MOC: $\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \pi 2p_x^2 = \pi 2p_y^2, \sigma 2p_z, \pi^* 2p_x = \pi^* 2p_y, \sigma^* 2p_z$

B.O. = $(N_b - N_a) / 2 = (8 - 4) / 2 = 2$

Magnetic Nature: It is diamagnetic in nature due to absence of unpaired electrons in molecular orbitals.



11. N_2^+ Molecular ion: It is formed by the combination of N atom and N^+ ion.

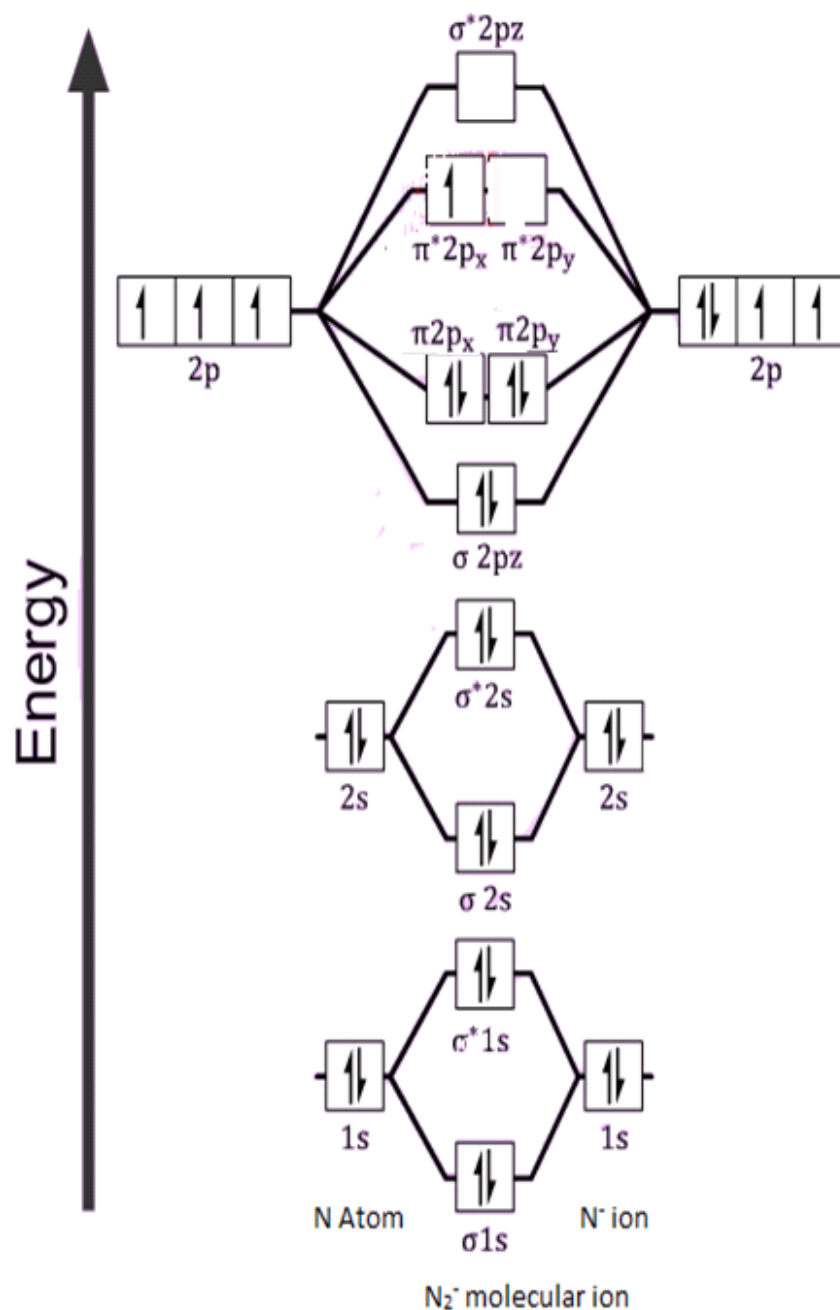
N atom + N^+ ion = N_2^+ molecular ion ($1s^2, 2s^2, 2p^3 + 1s^2, 2s^2, 2p^4$)

Total number of electrons in N_2^+ molecular ion = $7 + 8 = 15$

MOC: $\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \sigma 2p_z^2, \pi 2p_x^2 = \pi 2p_y^2, \pi^* 2p_x^1 = \pi^* 2p_y^1, \sigma^* 2p_z$

B.O. = $(N_b - N_a) / 2 = (10 - 5) / 2 = 2.5$

Magnetic Nature: It is paramagnetic in nature due to presence of unpaired electrons in molecular orbitals.



12. N₂²⁻ Molecular ion: It is formed by the combination of two N⁺ ions.

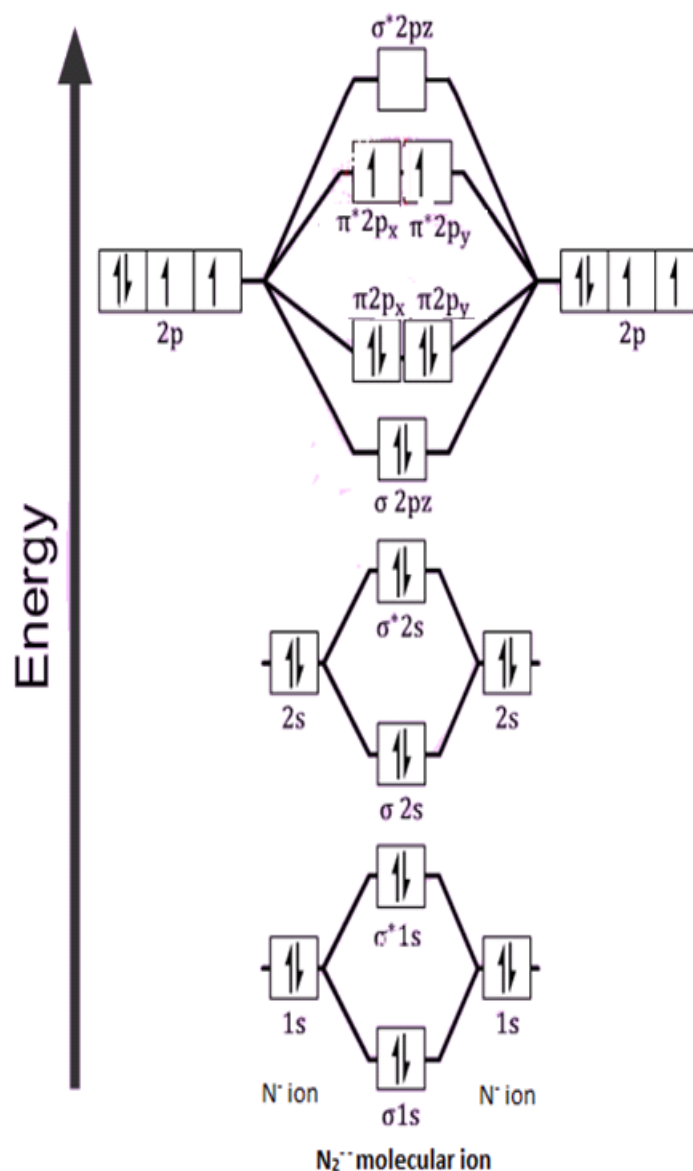
N⁺ ion + N⁺ ion = N₂²⁻ molecular ion (1s², 2s², 2p⁴ + 1s², 2s², 2p⁴)

Total number of electrons in N₂²⁻ molecular ion = 8 + 8 = 16

MOC: σ1s², σ*1s², σ2s², σ*2s², σ2pz², π2px² = π2py², π*2px¹ = π*2py¹, σ*2pz

B.O. = (N_b - N_a)/2 = (10 - 6)/2 = 2

Magnetic Nature: It is paramagnetic in nature due to presence of unpaired electrons in molecular orbitals.



13. O₂ Molecule: It is formed by the combination of two Oxygen atoms.

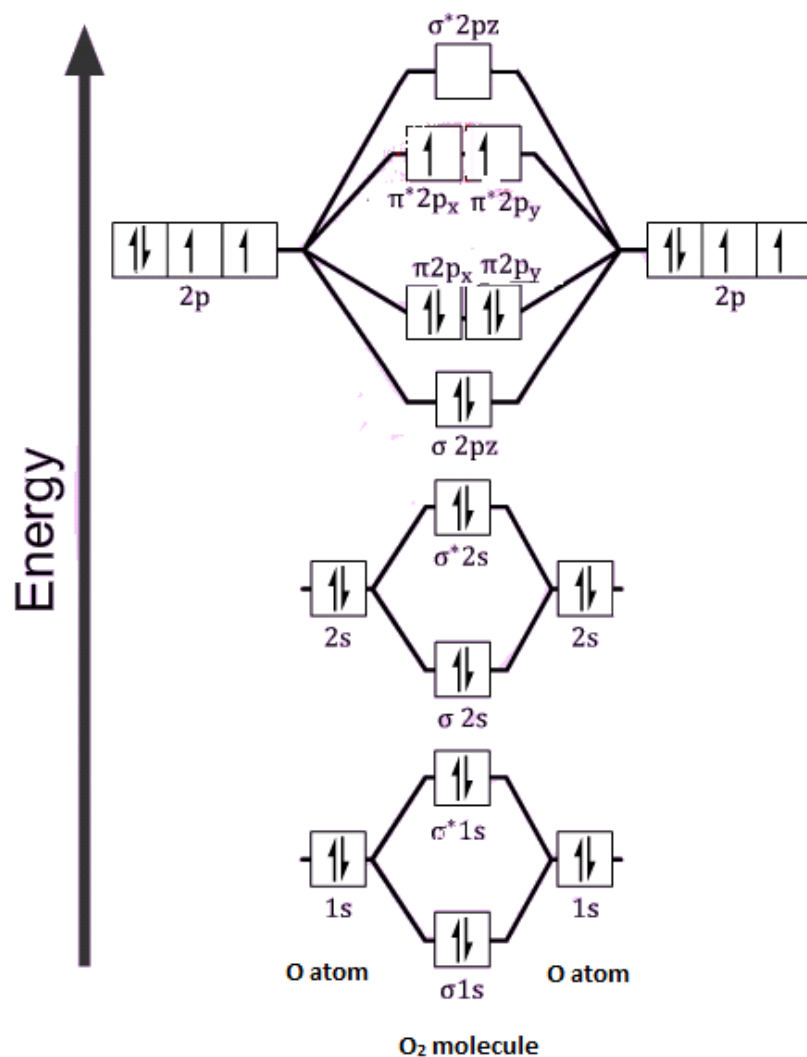
O atom + O atom = O₂ molecule ($1s^2, 2s^2, 2p^4 + 1s^2, 2s^2, 2p^4$)

Total number of electrons in O₂ molecule = 8 + 8 = 16

MOC: $\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \sigma 2p_z^2, \pi 2p_x^2 = \pi 2p_y^2, \pi^* 2p_x^1 = \pi^* 2p_y^1, \sigma^* 2p_z$

B.O. = $(N_b - N_a) / 2 = (10 - 6) / 2 = 2$

Magnetic Nature: It is paramagnetic in nature due to presence of unpaired electrons in molecular orbitals.



14. O_2^+ Molecular ion: It is formed by the combination of O atom and O^+ ion.

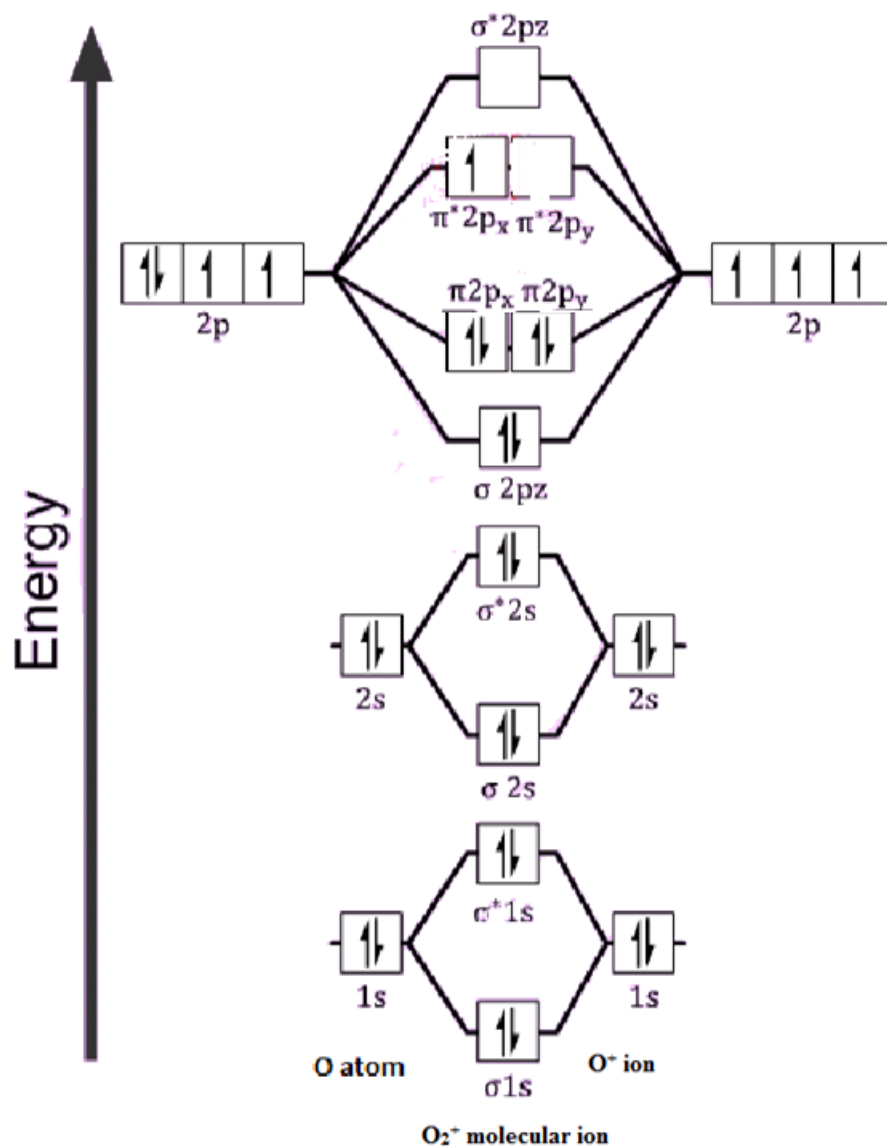
O atom + O^+ ion = O_2^+ molecular ion ($1s^2, 2s^2, 2p^4 + 1s^2, 2s^2, 2p^3$)

Total number of electrons in O_2^+ molecular ion = $8 + 7 = 15$

MOC: $\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \sigma 2p_z^2, \pi 2p_x^2 = \pi 2p_y^2, \pi^* 2p_x^1 = \pi^* 2p_y^1, \sigma^* 2p_z$

B.O. = $(N_b - N_a) / 2 = (10 - 5) / 2 = 2.5$

Magnetic Nature: It is paramagnetic in nature due to presence of unpaired electrons in molecular orbitals.



15. O₂⁺⁺ Molecular ion: It is formed by the combination of two O⁺ ions.

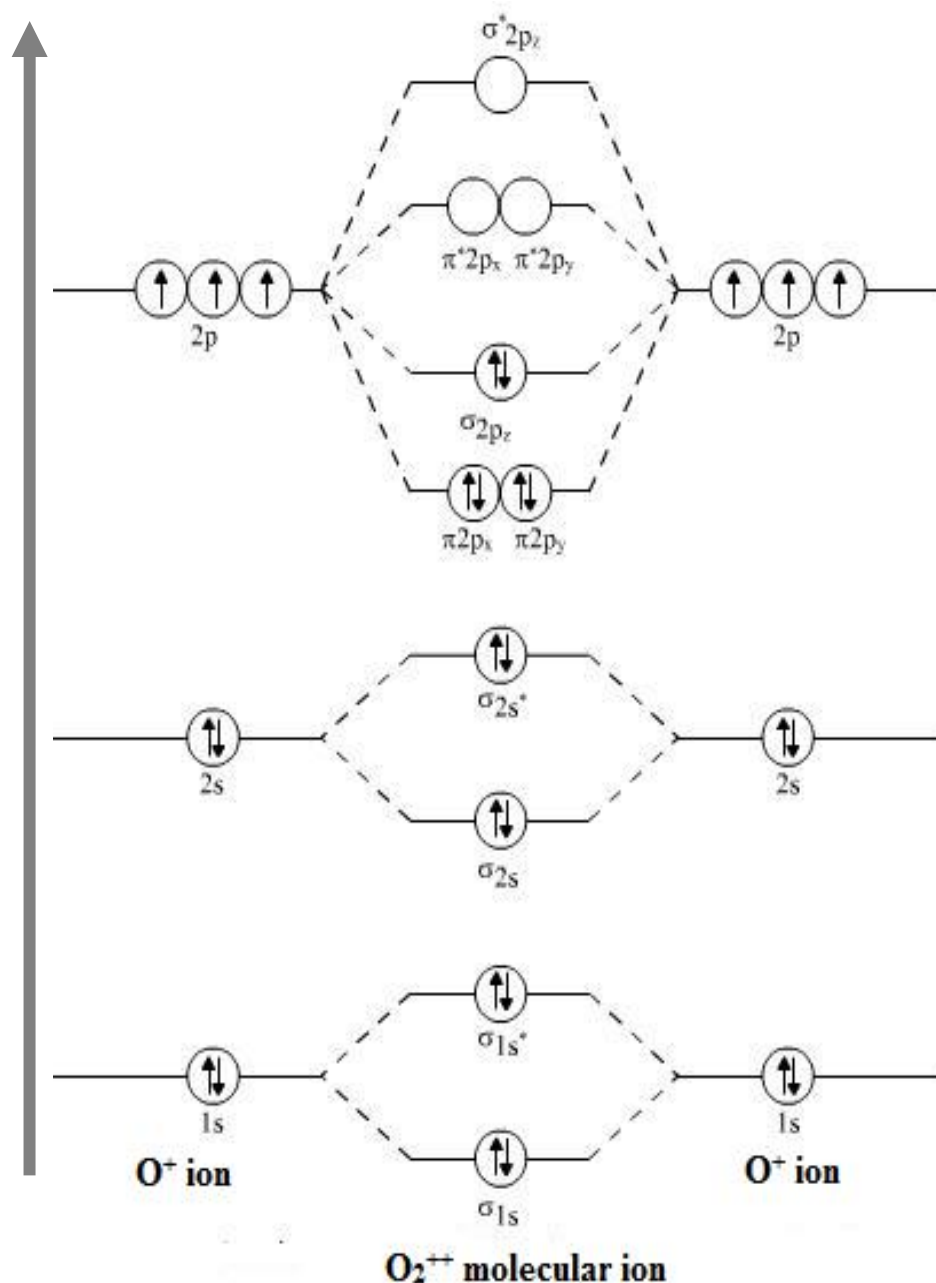
O⁺ ion + O⁺ ion = O₂⁺⁺ molecular ion (1s², 2s², 2p³ + 1s², 2s², 2p³)

Total number of electrons in O₂⁺⁺ molecular ion = 7 + 7 = 14

MOC: σ1s², σ*1s², σ2s², σ*2s², π2p_x² = π2p_y², σ2p_z², π*2p_x = π*2p_y, σ*2p_z

B.O. = (N_b - N_a) / 2 = (10 - 4) / 2 = 3

Magnetic Nature: It is diamagnetic in nature due to absence of unpaired electrons in molecular orbitals.



16. O₂⁻ Molecular ion (Superoxide ion): It is formed by the combination of O atom and O⁻ ion.

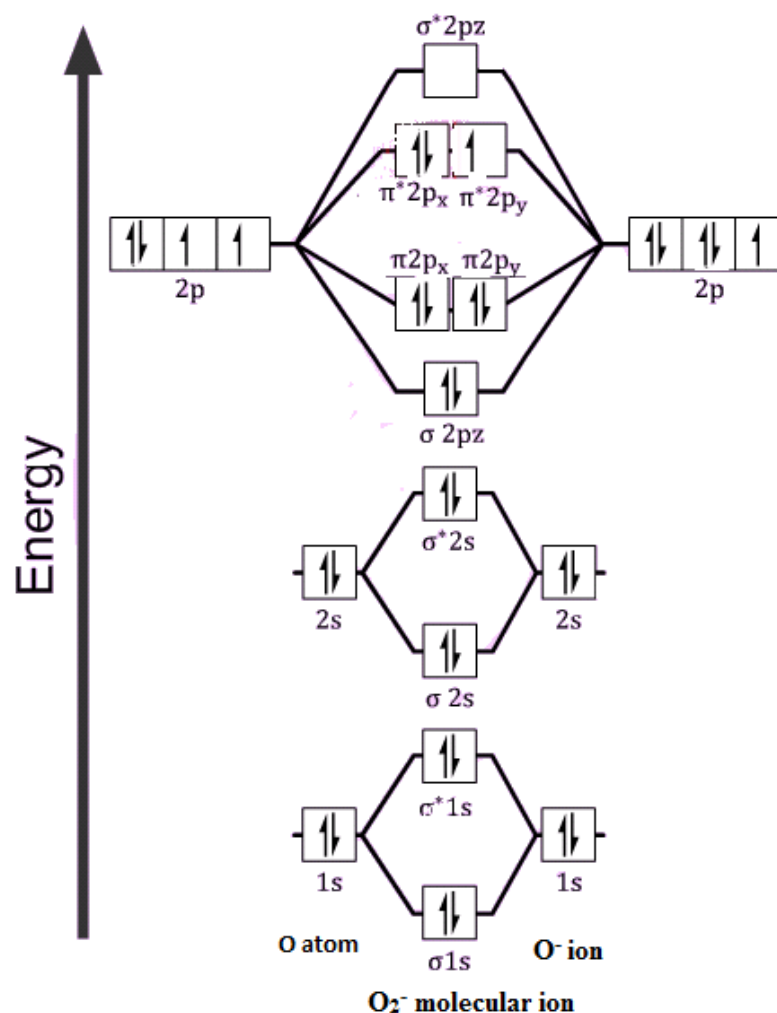
O atom + O⁻ ion = O₂⁻ molecular ion ($1s^2, 2s^2, 2p^4 + 1s^2, 2s^2, 2p^5$)

Total number of electrons in O₂⁻ molecular ion = 8 + 9 = 17

MOC: $\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \sigma 2p_z^2, \pi 2p_x^2 = \pi 2p_y^2, \pi^* 2p_x^1 = \pi^* 2p_y^1, \sigma^* 2p_z$

B.O. = $(N_b - N_a) / 2 = (10 - 7) / 2 = 1.5$

Magnetic Nature: It is paramagnetic in nature due to presence of unpaired electrons in molecular orbitals.



17. O₂²⁻ Molecular ion (Peroxide ion): It is formed by the combination of two O⁺ ions.

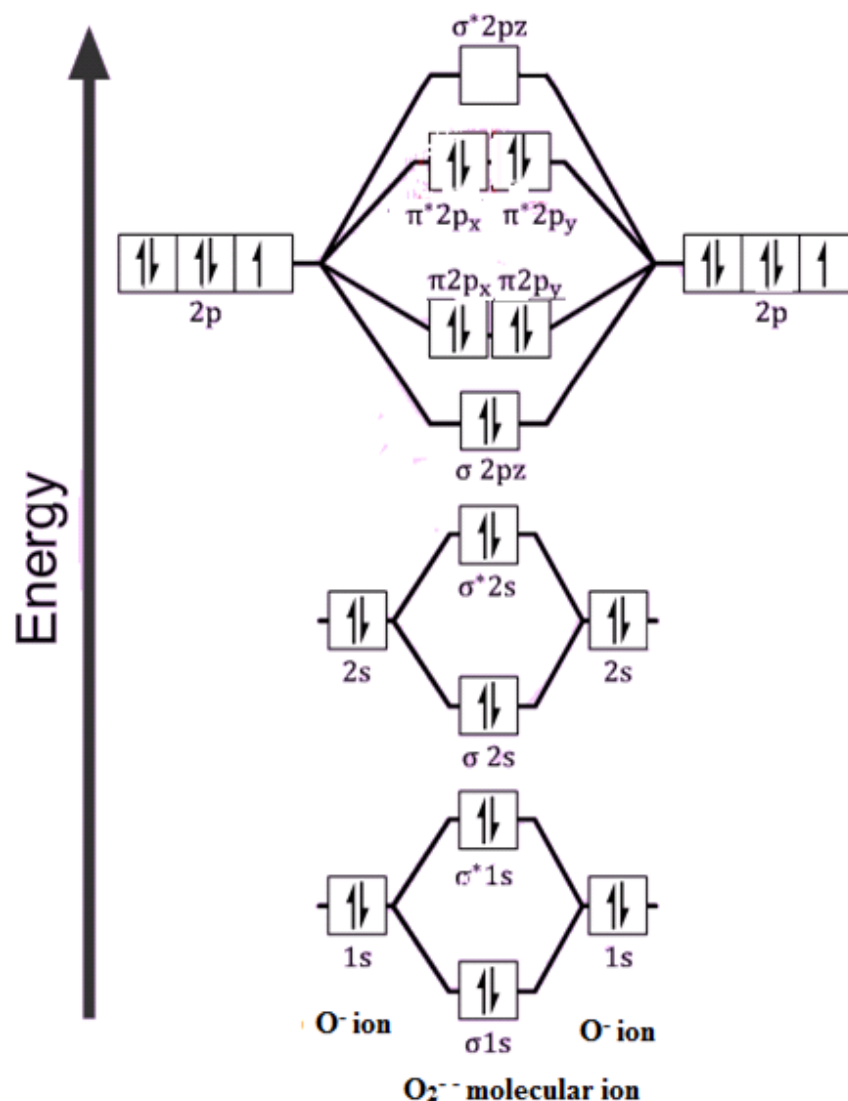
O⁺ ion + O⁺ ion = O₂²⁻ molecular ion ($1s^2, 2s^2, 2p^5 + 1s^2, 2s^2, 2p^5$)

Total number of electrons in O₂²⁻ molecular ion = 9 + 9 = 18

MOC: $\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \sigma 2p_z^2, \pi 2p_x^2 = \pi 2p_y^2, \pi^* 2p_x^2 = \pi^* 2p_y^2, \sigma^* 2p_z$

B.O. = $(N_b - N_a) / 2 = (10 - 8) / 2 = 1$

Magnetic Nature: It is diamagnetic in nature due to absence of unpaired electrons in molecular orbitals.



18. F₂ Molecule: It is formed by the combination of two Fluorine atoms.

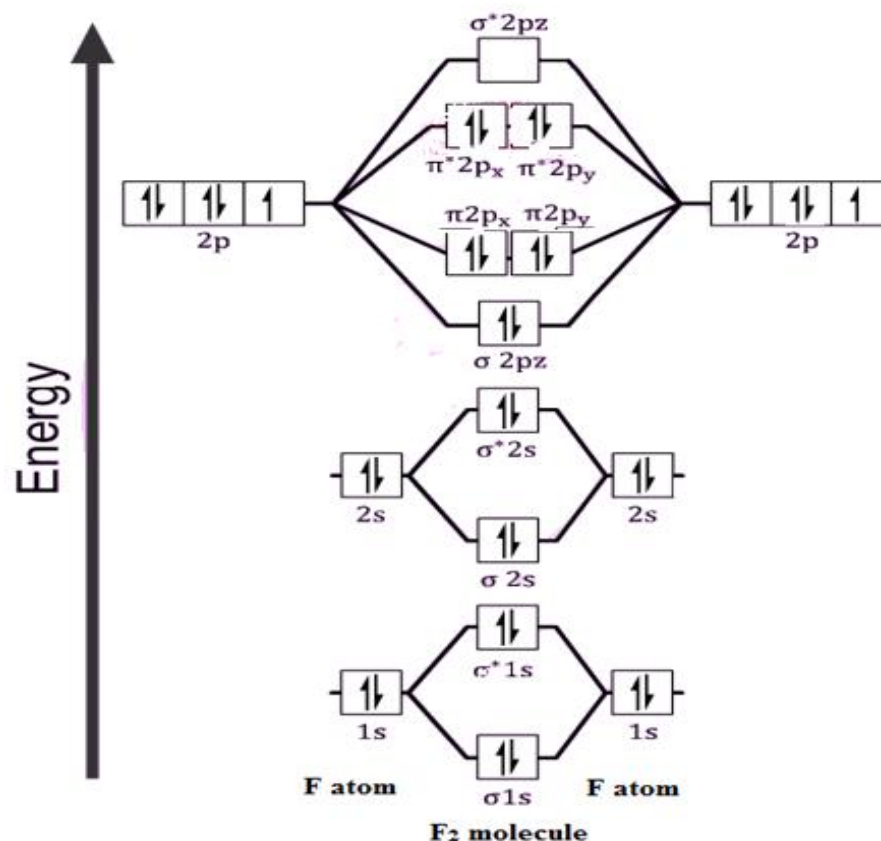
F atom + F atom = F₂ molecule ($1s^2, 2s^2, 2p^5 + 1s^2, 2s^2, 2p^5$)

Total number of electrons in F₂ molecule = 9 + 9 = 18

MOC: $\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \sigma 2p_z^2, \pi 2p_x^2 = \pi 2p_y^2, \pi^* 2p_x^2 = \pi^* 2p_y^2, \sigma^* 2p_z$

B.O. = $(N_b - N_a) / 2 = (10 - 8) / 2 = 1$

Magnetic Nature: It is diamagnetic in nature due to absence of unpaired electrons in molecular orbitals.



19. Ne₂ molecule: It is formed by the combination of two neon atoms.

Ne atom + Ne atom = Ne₂ molecule

Total number of electrons in Ne₂ molecule = 10 + 10 = 20

MOC: $\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \sigma 2p_z^2, \pi 2p_x^2 = \pi 2p_y^2, \pi^* 2p_x^2 = \pi^* 2p_y^2, \sigma^* 2p_z^2$

B.O. = $(N_b - N_a)/2 = (10 - 10)/2 = 0$

Because B.O. is zero so Ne₂ molecule does not exist.

EXAMPLES OF HETERONUCLEAR DIATOMIC MOLECULES AND MOLECULAR IONS:

1. CO Molecule: It is formed by the combination of C and O atoms.

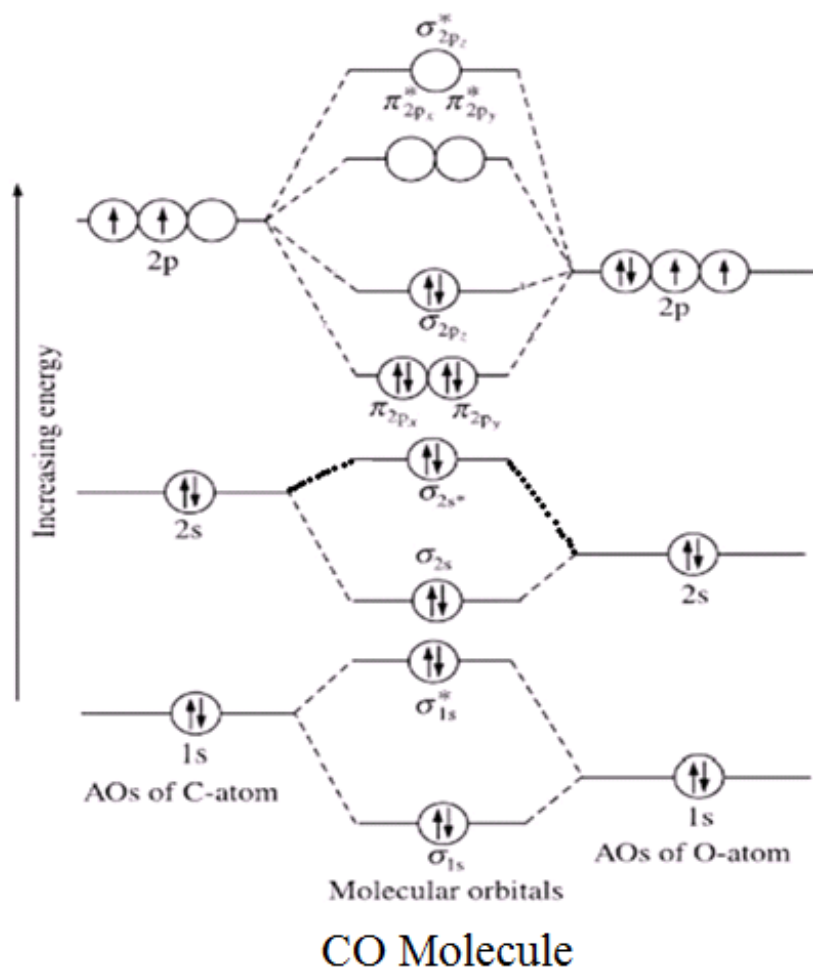
C atom + O atom = CO molecule ($1s^2, 2s^2, 2p^2 + 1s^2, 2s^2, 2p^4$)

Total number of electrons in CO molecule = 6 + 8 = 14

MOC: $\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \pi 2p_x^2 = \pi 2p_y^2, \sigma 2p_z^2, \pi^* 2p_x = \pi^* 2p_y, \sigma^* 2p_z$

B.O. = $(N_b - N_a)/2 = (10 - 4)/2 = 3$

Magnetic Nature: It is diamagnetic in nature due to absence of unpaired electrons in molecular orbitals.



2. **CO⁺ Molecular ion:** It is formed by the combination of C atom and O⁺ ion.

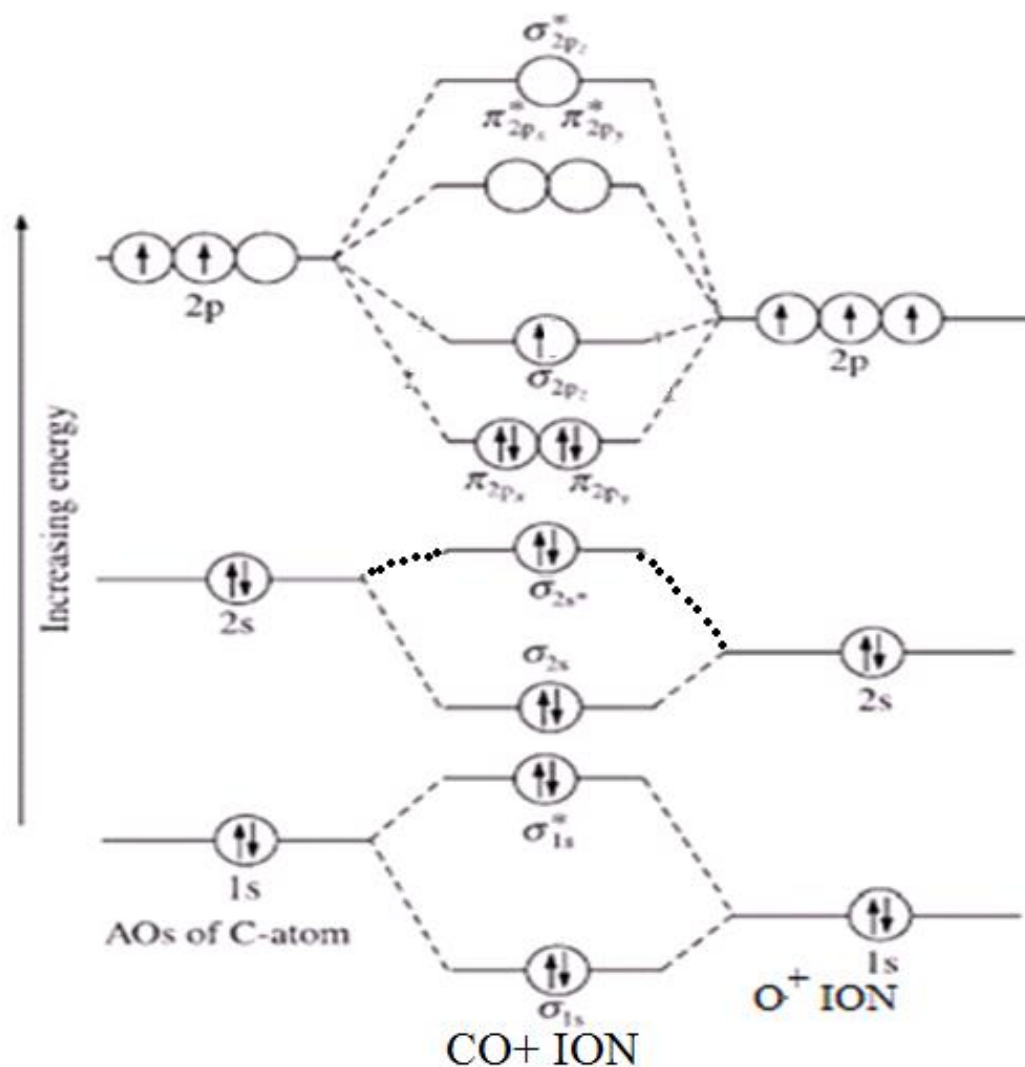
C atom + O⁺ ion = CO⁺ molecular ion ($1s^2, 2s^2, 2p^2 + 1s^2, 2s^2, 2p^3$)

Total number of electrons in CO⁺ molecular ion = 6 + 7 = 13

MOC: $\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \pi 2p_x^2 = \pi 2p_y^2, \sigma 2p_z^1, \pi^* 2p_x = \pi^* 2p_y, \sigma^* 2p_z$

B.O. = $(N_b - N_a) / 2 = (9 - 4) / 2 = 2.5$

Magnetic Nature: It is paramagnetic in nature due to presence of unpaired electrons in molecular orbitals.



3. **NO Molecule:** It is formed by the combination of N atom and O atom.

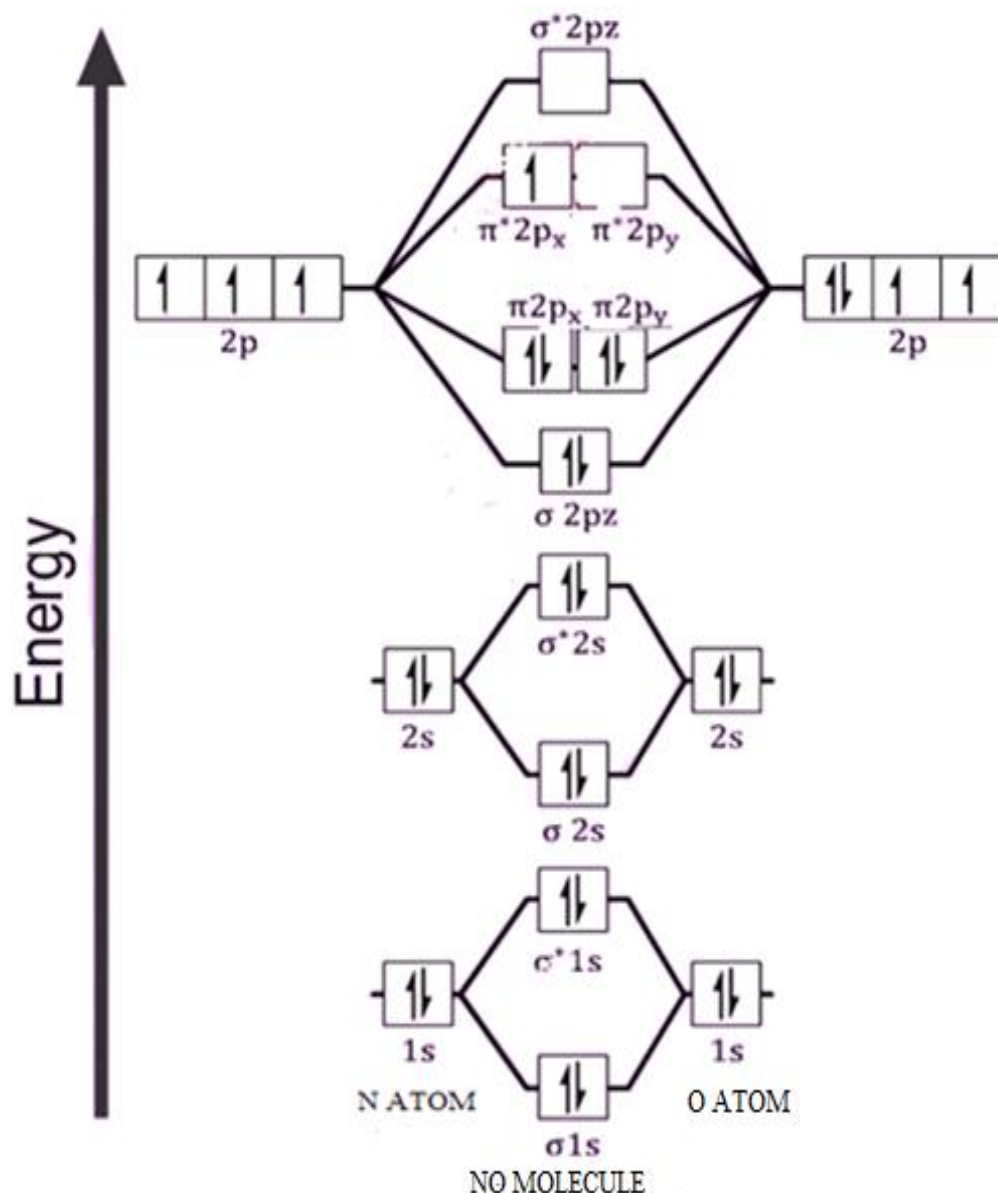
N atom + O atom = NO molecule ($1s^2, 2s^2, 2p^3 + 1s^2, 2s^2, 2p^4$)

Total number of electrons in NO molecule = $7 + 8 = 15$

MOC: $\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \sigma 2p_z^2, \pi 2p_x^2 = \pi 2p_y^2, \pi^* 2p_x^1 = \pi^* 2p_y^1, \sigma^* 2p_z$

B.O. = $(N_b - N_a) / 2 = (10 - 5) / 2 = 2.5$

Magnetic Nature: It is paramagnetic in nature due to presence of unpaired electrons in molecular orbitals.



4. **NO[•] Molecular ion:** It is formed by the combination of N atom and O[•] ion.

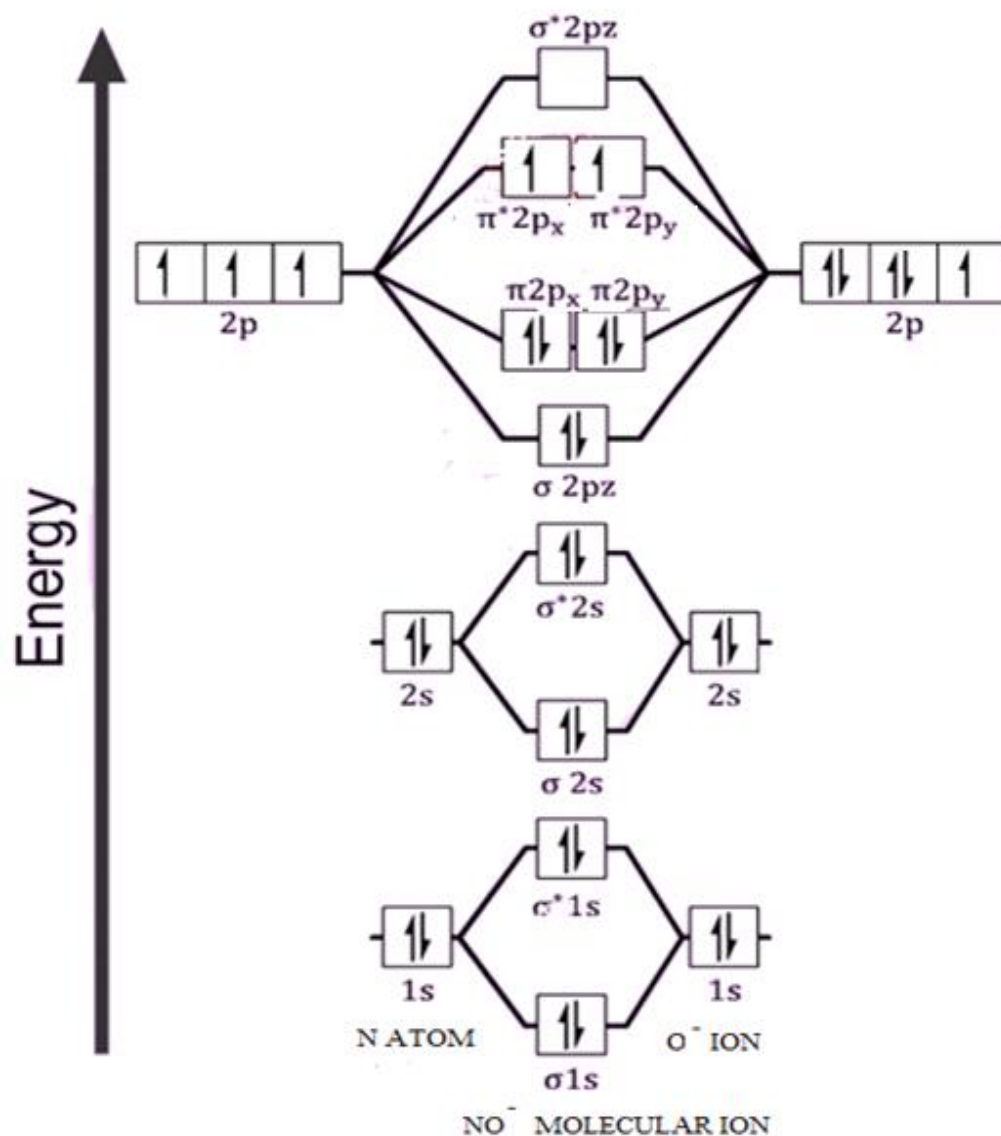
N atom + O[•] ion = NO[•] molecular ion ($1s^2, 2s^2, 2p^3 + 1s^2, 2s^2, 2p^5$)

Total number of electrons in NO[•] molecular ion = 7 + 9 = 16

MOC: $\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \sigma 2p_z^2, \pi 2p_x^2 = \pi 2p_y^2, \pi^* 2p_x^1 = \pi^* 2p_y^1, \sigma^* 2p_z$

B.O. = $(N_b - N_a) / 2 = (10 - 6) / 2 = 2$

Magnetic Nature: It is paramagnetic in nature due to presence of unpaired electrons in molecular orbitals.



5. **HF MOLECULE:** It is formed by the combination of H atom and F atom.

H^- atom + F^- atom = HF molecule ($1s^1 + 1s^2, 2s^2, 2p^5$)

(F atom = $1s^2, 2s^2, 2p_x^2, 2p_y^2, 2p_z^1$)

Total number of electrons in HF molecule = $1 + 9 = 10$

The energy of 1s atomic orbital of H atom becomes equal to 2p atomic orbital of F atom due to high electronegativity difference. So 1s atomic orbital of H atom only combine with $2p_z$ atomic orbital of F atom and form two molecular orbitals (σ_{sp} & σ^*_{sp}).

Magnetic Nature: It is diamagnetic in nature due to absence of unpaired electrons in molecular orbitals

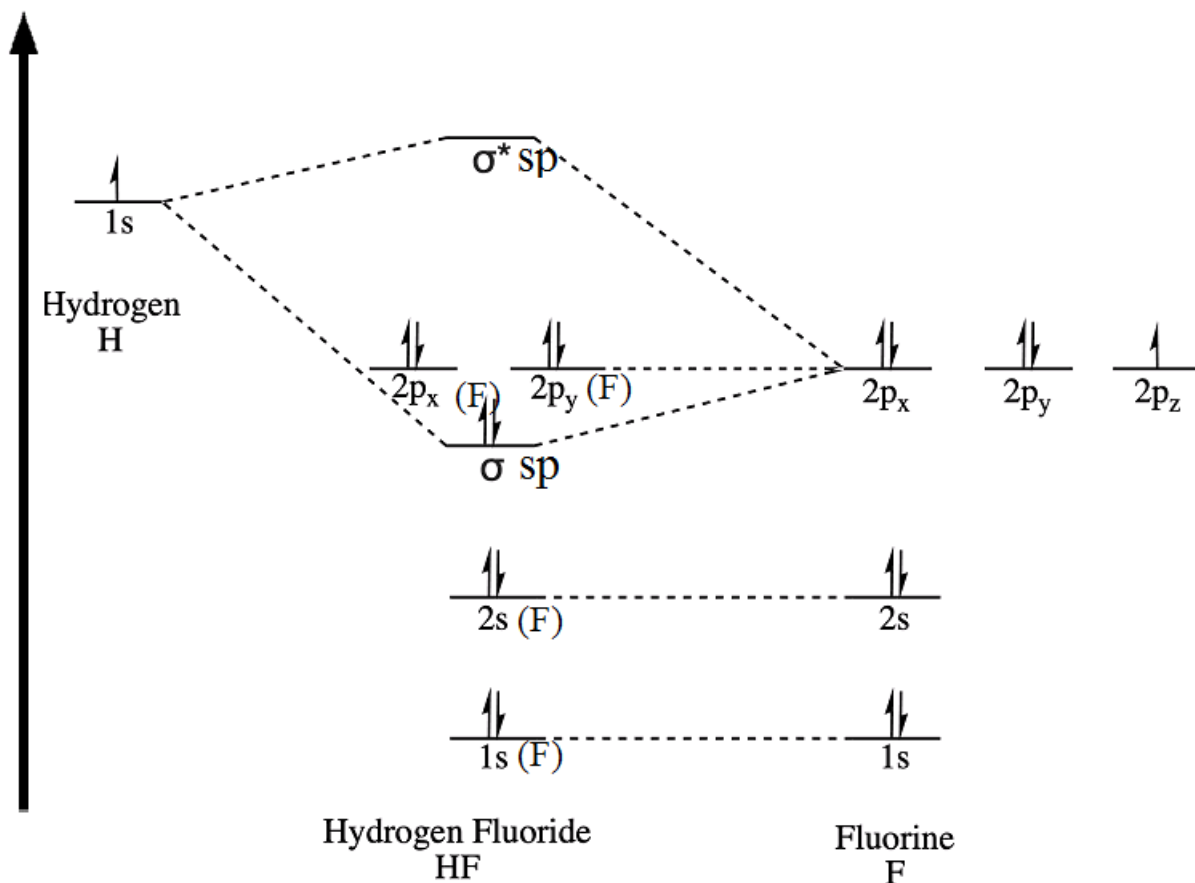
MOC: $1s^2, 2s^2, 2p_x^2 2p_y^2$, σsp^2 , $\sigma^* sp$

Non bonding

BMO

abmo

$$\text{B.O.} = (N_b - N_a)/2 = (2 - 0)/2 = 1 \quad (\text{H} - \text{F})$$



6. **HCl MOLECULE:** It is formed by the combination of H atom and Cl atom.

H- atom + **Cl-** atom = **HCl** molecule ($1s^1 + 1s^2, 2s^2, 2p^6, 3s^2 3p^5$)

(Cl atom = $1s^2, 2s^2, 2p^6, 3s^2, 3p_x^2, 3p_y^2, 3p_z^1$)

Total number of electrons in HCl molecule = 1 + 17 = 18

The energy of 1s atomic orbital of H atom becomes equal to 3p atomic orbital of Cl atom due to high electronegativity difference. So 1s atomic orbital of H atom only combine with $3p_z$ atomic orbital of Cl atom and form two molecular orbitals (σsp & $\sigma^* sp$).

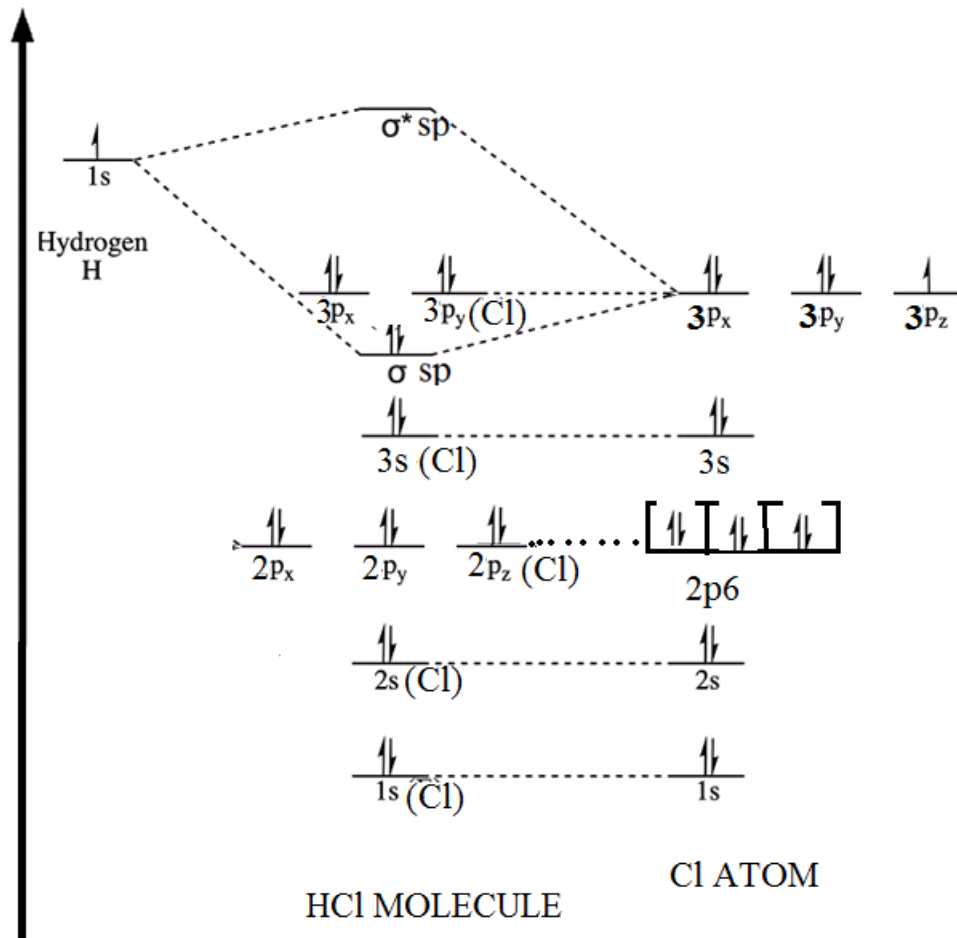
MOC: $1s^2, 2s^2, 2p^6, 3s^2, 3p_x^2, 3p_y^2$, σsp^2 , $\sigma^* sp$

Non bonding

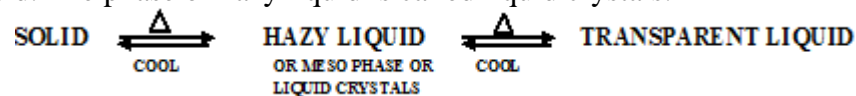
BMO

abmo

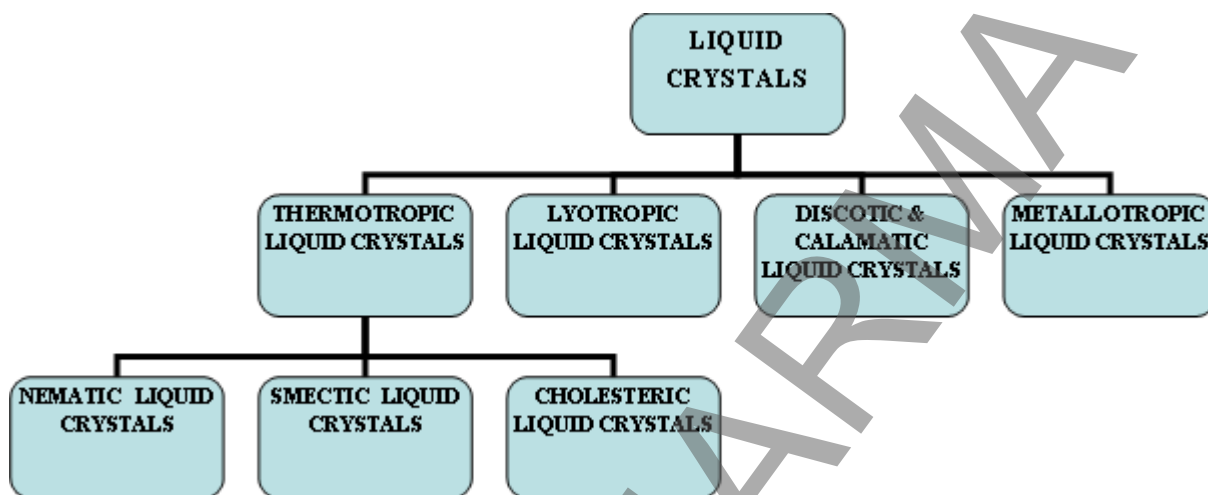
$$\text{B.O.} = (N_b - N_a)/2 = (2 - 0)/2 = 1 \quad (\text{H} - \text{Cl})$$



LIQUID CRYSTALS: Liquid crystals (LCs) are matter in a state which has properties between those of conventional liquids and those of crystalline solid. A liquid crystal may flow like a liquid, but its molecules may be oriented in a crystal-like way. It is also called mesophase or middle phase. When a solid is heated slowly it is converted into hazy liquid which on further heating converted into transparent liquid. The phase of hazy liquid is called liquid crystals.



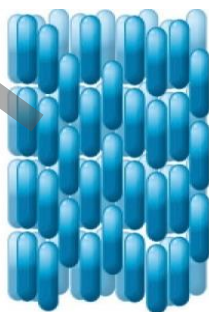
Types of Liquid Crystals: Generally liquid crystals can be divided into following parts.



1. Thermotropic liquid crystals: Those liquid crystals which are based on temperature range are called thermotropic liquid crystals.

These are further divided into three parts

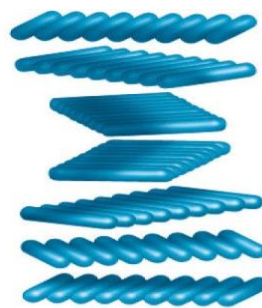
a. Nematic liquid crystals: The word nema is taken from the Greek word Nema which means thread like. Those liquid crystals which have thread like structure are called nematic liquid crystals. In these liquid crystals organic molecules have no positional order, but they self-align to have long-range directional order with their long axes roughly parallel.



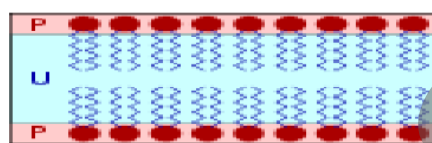
b. Smectic liquid crystals: The word "smectic" originates from the Latin word "smecticus", meaning cleaning, or having soap-like properties. Those liquid crystals which have soap like structure are called smectic liquid crystals. In these liquid crystals organic molecules are positionally ordered along one direction.



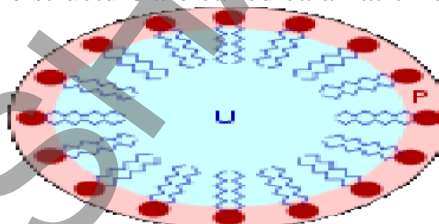
c. Cholesteric liquid crystals: Those liquid crystals which have cholesterol like structure are called cholesteric liquid crystals. In these liquid crystals organic molecules are arranged in layers with different orientation in each layer.



2. **Lyotropic liquid crystals:** Those liquid crystals which are based on concentration are called lyotropic liquid crystals. For Example: Micelles
3. **Discotic and calamatic liquid crystals:** Those liquid crystals which have disk like structure are called discotic liquid crystals. Those liquid crystals which have rod like structure are called calamatic liquid crystals.



CALAMATIC OR ROD LIKE LIQUID CRYSTALS



DISCOTIC LIQUID CRYSTALS

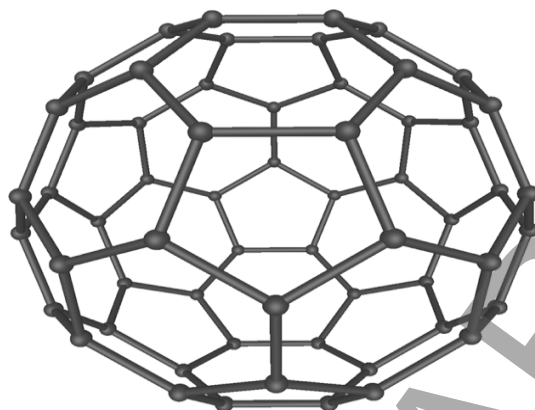
4. **Metallotropic liquid crystals:** Some of the low melting inorganic compounds such as ZnCl_2 are formed metallotropic liquid crystals.

Applications of Liquid Crystals:

1. Liquid crystals are used for making LCD's.
2. These are used for making digital calculators, laptops, computers and mobile screens.
3. These are used for making digital thermometers.
4. These are used in thermography for detecting tumors.
5. These are used for making electro optical devices.

FULLERENE: It is an allotrope of carbon. It was discovered by H.Kroto and Richard E. Smalley in 1985. Its structure was proposed by architect Buckminster Fuller, so it is also known as Buckminster fullerene. It consists of hollow spherical soccer ball like structure so it is also called Bucky ball.

Structure of Fullerene: It is represented by C_{60} . In the structure of fullerene each carbon atom is sp^2 hybridized and contains pentagons and hexagons. 1 molecule C_{60} consists of 20 hexagons and 12 pentagons. They are arranged in truncated icosahedrons structure in such a way that two pentagons never share their wall.

**Preparation:**

1. It is prepared by vaporizing the graphite rod in the inert atmosphere of argon or helium . As a result a mixture of fullerenes is obtained which can be separated by chromatography or fractional distillation.
2. It is also prepared by benzene –oxygen flame in a specially designed helium atmosphere.

Properties of Fullerene:

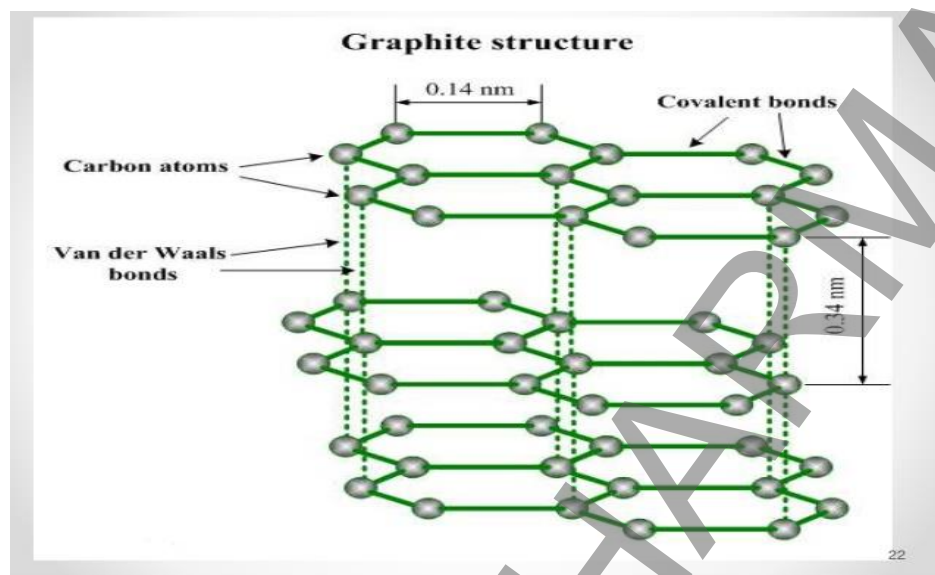
1. It is a mustard colored crystalline solid.
2. It gives magenta colored solution on dissolving in benzene.
3. The colored of fullerene film changes from dark brown to black as the thickness of film increases.

Applications of Fullerene:

1. It is used for making carbon nano tubes and nano wires.
2. It is used for making super conductors.
3. It is used for detecting cancer cells.
4. It is used to inhibited HIV protease.
5. It is used for making ferromagnets.
6. It is used for making electronic and optical devices.

GRAPHITE: Graphite is an allotrope of carbon. It has 2 dimension layers like structure. It is also called sandwich like structure.

Structure of Graphite: In the structure of graphite each carbon atom is sp^2 hybridized and hexagonally arranged in layers. In the layer each carbon atom is linked to three other carbon atoms in the same plain through covalent bonds. The fourth valance of carbon atom is satisfied by weak van der Walls forces between two layers. The C-C bond length 0.142 nm within the layer and distance between two layers is 0.34 nm.



Types of graphite: Generally there are two types of graphite.

1. **α - Graphite:** In α - graphite the layers are arranged in the sequence of ABAB arrangement.
2. **β - Graphite:** In β - graphite the layers are arranged in the sequence of ABC- ABC.

Properties of graphite: It is very soapy to touch, non-inflammable. It is soft in nature and conductor of electricity.

Uses of Graphite:

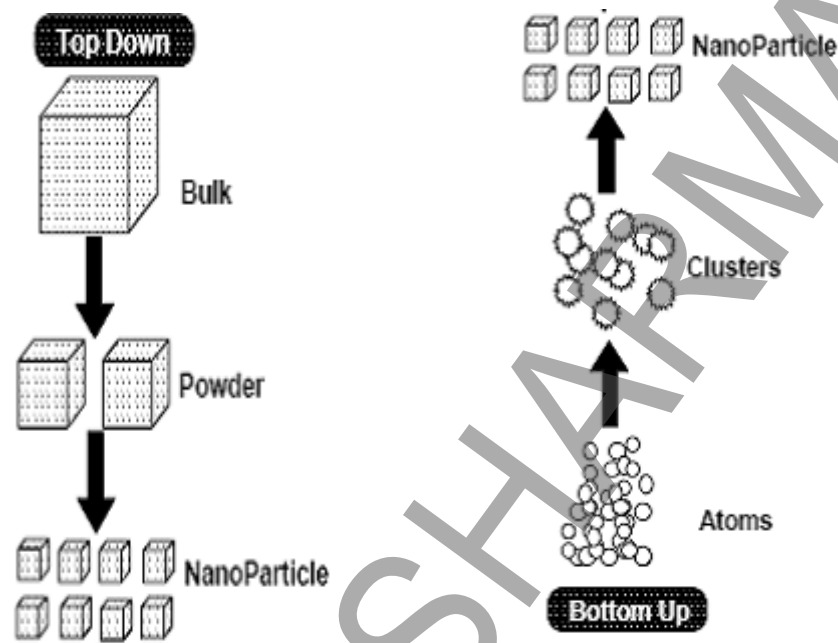
1. It is used as solid lubricants.
2. It is used for making electrodes.
3. It is used for making metallurgical crucibles.
4. It is used for making pencil lead.
5. It is used for making moderator rods in nuclear power plant.

NANOMATERIALS: All the materials (i.e. organic, inorganic, ceramic, metals, nonmetals etc.) which lies in nanorange 1 nm to 100 nm are called nanomaterials.

For Example: Micelles, Fullerene, Carbon nanotube etc.

Methods of Preparation of nanomaterials: Nanomaterials can be prepared by following methods

1. **Top Down approach:** In this method particles of large size are break down physically or mechanically into particles of nanorange (1nm to 100nm).
2. **Bottom up approach:** In this method particles of very small size are condensed into particles of nanorange (1nm to 100nm).

**Applications of Nanomaterials:**

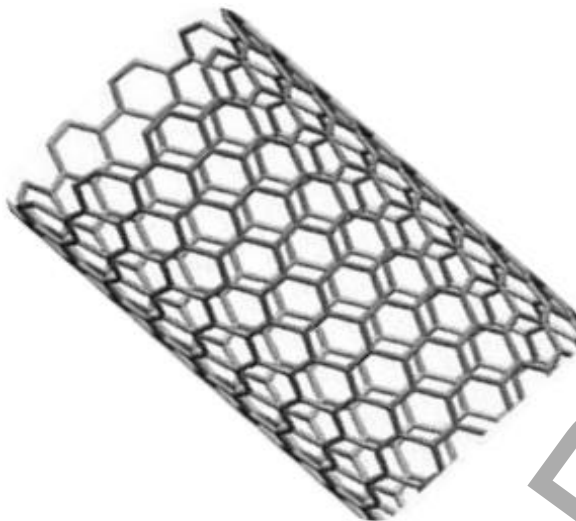
1. It is used for making super conductors.
2. It is used for making carbon nanotubes.
3. It is used for making nanowires.
4. It is used for making smart materials.
5. It is used for making optical sensors.
6. It is used for making special medicines.

NANOSCIENCE OR NANOTECHNOLOGY: The branch of science which deals with the study of all materials lies in the nanorange i.e. 1 nm to 100 nm is called nanoscience or nanotechnology.

Nanoscience and nanotechnology are the study and application of extremely small things and can be used across all the other science fields, such as chemistry, biology, physics, materials science, and engineering.

CARBON NANOTUBES (CNT): Carbon nanotubes are a form of carbon, similar to graphite found in pencils. They are hollow cylindrical tubes and are 10,000 times smaller than human hair, but stronger than steel. They are also good conductors of electricity and heat, and have a very large surface area.

When graphene sheet is fold cylindrically then we get a cylindrical hollow tube like structure, which is called carbon nanotube.



Generally there are two types of carbon nanotubes:

1. **SWCNT:** Single wall carbon nanotube.
2. **MWCNT:** Multi wall carbon nanotube.

Applications of Carbon Nanotubes:

1. It is used for making super conductors.
2. It is used for making nanowires.
3. It is used for making smart materials.
4. It is used for making optical sensors.

GREEN CHEMISTRY: Green chemistry is the design of chemical products and processes that reduce or eliminate the use or generation of hazardous substances.

Green chemistry applies across the life cycle of a chemical product, including its design, manufacture, use, and ultimate disposal.

Green chemistry can also be described as

- Sustainable chemistry.
- Chemistry that is benign by design.
- Pollution prevention at the molecular level.
- All of the above.
- Focus on processes and products that reduce or eliminate the use of polluting substances

Any synthesis, whether performed in teaching, laboratories or industries should create none or minimum by-products which pollute the atmosphere.

THE BENEFITS OF GREEN CHEMISTRY:

- Economical
- Energy efficient
- Lowers cost of production and regulation
- Less wastes
- Fewer accidents
- Safer products

- Healthier workplaces and communities
- Protects human health and the environment.

WHY DO WE NEED GREEN CHEMISTRY?

- Chemistry is undeniably a very prominent part of our daily lives.
- Chemical developments bring new environmental problems and harmful unexpected side effects, which result in the need for 'greener' chemical products. Eg. DDT.
- Green chemistry looks at pollution prevention on the molecular scale. It is an extremely important area of Chemistry due to the importance of Chemistry in our world today and the implications it can show on our environment.
- The Green Chemistry program supports the invention of more environmentally friendly chemical processes which reduce or even eliminate the generation of hazardous substances.

This program works very closely with the twelve principles of Green Chemistry.

12 Principles of Green Chemistry:

- **Prevention:** Design chemical syntheses to prevent waste. It is better to prevent waste than to treat or clean up waste after it is formed.
- **Atom Economy:** Synthetic methods should be designed to maximize the incorporation of all materials used in the process into the final product.
- **Less Hazardous Chemical Synthesis:** Whenever practicable, synthetic methodologies should be designed to use and generate substances that possess little or no toxicity to human health and the environment.
- **Designing Safer Chemicals:** Chemical products should be designed to preserve efficacy of the function while reducing toxicity.
- **Safer Solvents and Auxiliaries:** The use of auxiliary substances (solvents, separation agents, etc.) should be made unnecessary whenever possible and, when used, innocuous (harmless)
- **Design for Energy Efficiency:** Energy requirements should be recognized for their environmental and economic impacts and should be minimized. Synthetic methods should be conducted at ambient temperature and pressure.
- **Use of Renewable Feed stocks:** A raw material or feedstock should be renewable rather than depleting whenever technically and economically practical.
- **Reduce Derivatives:** Unnecessary derivatization (blocking group, protection/deprotection, and temporary modification of physical/chemical processes) should be avoided whenever possible.
- **Catalysis:** Catalytic reagents (as selective as possible) are superior to stoichiometric reagents.
- **Design for Degradation:** Chemical products should be designed so that at the end of their function they do not persist in the environment and instead break down into innocuous degradation products.
- **Real-time Analysis for Pollution Prevention:** Analytical methodologies need to be further developed to allow for real-time in-process monitoring and control prior to the formation of hazardous substances.
- **Inherently Safer Chemistry for Accident Prevention:** Substance and the form of a substance used in a chemical process should be chosen so as to minimize the potential for chemical accidents, including releases, explosions, and fires.

Synthesis of Adipic Acid: Adipic acid is a very important starting material for Nylon-6,6 and cakehole (which is used in the pharmaceutical and pesticide industries).

The industrial production of Adipic acid used benzene as a starting material. Benzene is one of the basic chemicals for industrial reactions and a solvent. It is known that derives mainly from the refining processes of the petrochemical industry.

Benzene is also known for its carcinogenic properties (it causes leukemia to highly exposed workers). Afterwards the starting material became cyclohexanone or a mixture of cyclohexanone and cyclohexanol.

For the oxidation process it was used nitric acid, producing toxic fumes of nitric oxides, NO_x, which are also contributors to the greenhouse effect and the destruction of the ozone layer in the stratosphere.

It was Inevitable that the method had to be changed again with more environmentally benign reactions.

Finally, chemical engineers and synthetic organic chemists researched for alternatives. The “greener” method of adipic acid uses a new generation of catalysts.

The starting chemical is cyclohexene and its oxidation is performed by 30% hydrogen peroxide (H₂O₂). The catalyst is dissolved in a special organic solvent (Aliquat 336). The catalyst is a salt of the metal Wolframs or Tungsten (W) [Tungsten catalysts (Na₂WO₄/KHSO₄/ Aliquat 336).

