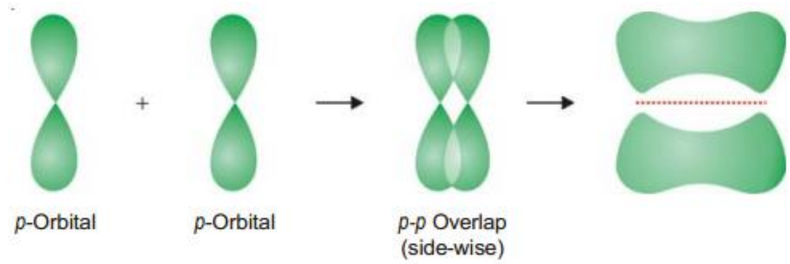


Differences Between Sigma and Pi bonds

Sigma (σ) bond	Pi (π) Bond
1. It is formed by *end to end* overlapping of half filled atomic orbitals.	1. It is formed by the sidewise overlapping of half filled *p*-orbitals only.
2. Overlapping takes place along internuclear axis.	2. Overlapping takes place perpendicular to internuclear axis.
3. The extent of overlapping is large and bond formed is *stronger*.	3. The extent of overlapping is small and bond formed is *weaker*.
4. The molecular orbital formed as a result of overlapping is symmetrical about the internuclear axis.	4. The molecular orbital formed as a result of overlapping consists of two lobes above and below the internuclear axis.
5. There is free rotation about σ bond and no geometrical isomers are possible.	5. There is no free rotation about π bond and geometrical isomers are possible.
6. The bond can be present alone.	6. The bond is always formed in addition to sigma (σ) bond.
7. *s* and *p* orbitals can participate in the formation of σ bond.	7. Only *p*-orbitals participate in the formation of π bond.

2. MOLECULAR ORBITAL THEORY

Molecular orbital theory (MOT) was developed by Hund and Milliken in 1927 and extended later by Lennard-Jones in 1929. According to molecular orbital theory (MOT);

1. The atomic orbitals overlap to form molecular orbitals and the number of atomic orbitals is always equal to the number of molecular orbitals.

2. Half molecular orbitals are lower in energy called bonding molecular orbitals. Half molecular orbitals are higher in energy called anti bonding molecular orbitals.

3. Bonding molecular orbitals are represented as sigma (σ) or pi(л) and anti-bonding molecular orbitals are represented as sigma star(σ^*) or pi star(л*).

4. These molecular orbitals are filled up according to Aufbau principle and Hund's rule.

5. The increasing order of energy of molecular orbitals is;

Diagram

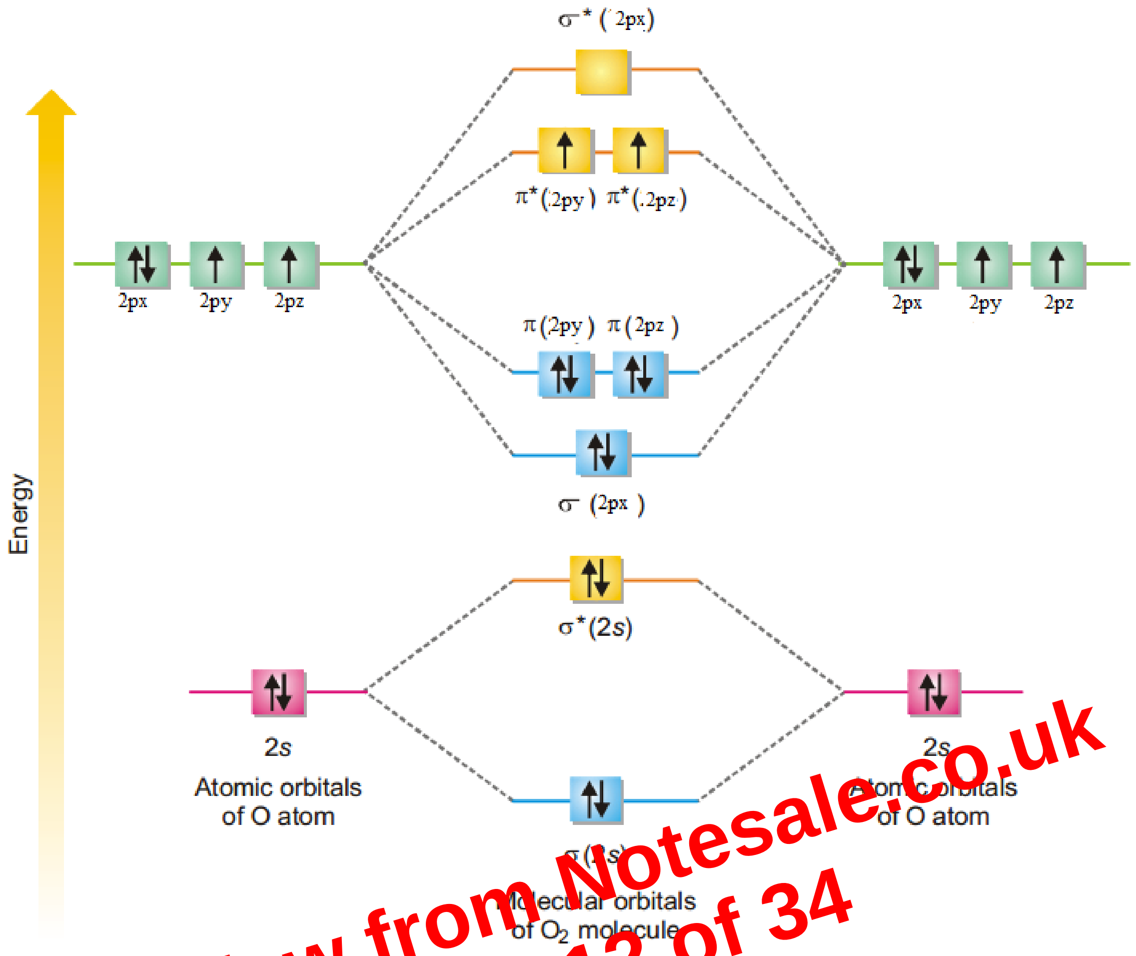


Fig: Molecular orbital diagram of O_2 molecule

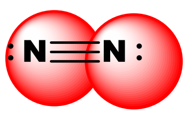
4. Nitrogen(N_2) molecule

Nitrogen (N) has electronic configuration $1s^2$, $2s^2$, $2px^1$, $2py^1$, $2pz^1$. These atomic orbitals of two nitrogen atom combine to form molecular orbitals. Nitrogen (N_2) molecule has the following configuration which can be represented as;

N ($1s^2$, $2s^2$, $2px^1$, $2py^{1,}$ $2pz^1$) + N($1s^2$, $2s^2$, $2px^1$, $2py^1$, $2pz^1$) $\longrightarrow$

N_2[($C2s^2$), (σ^*2s^2), $\sigma2px^2$, л$2py^2$, л$2pz^2$, σ^* $2px^0$, л$^*2py^0$, л$^*2pz^0$]

Bond order = 8-2/2 = 6/2 = 3, it means that Nitrogen (N_2) molecule contain triple bond. e.g.,



Diagram

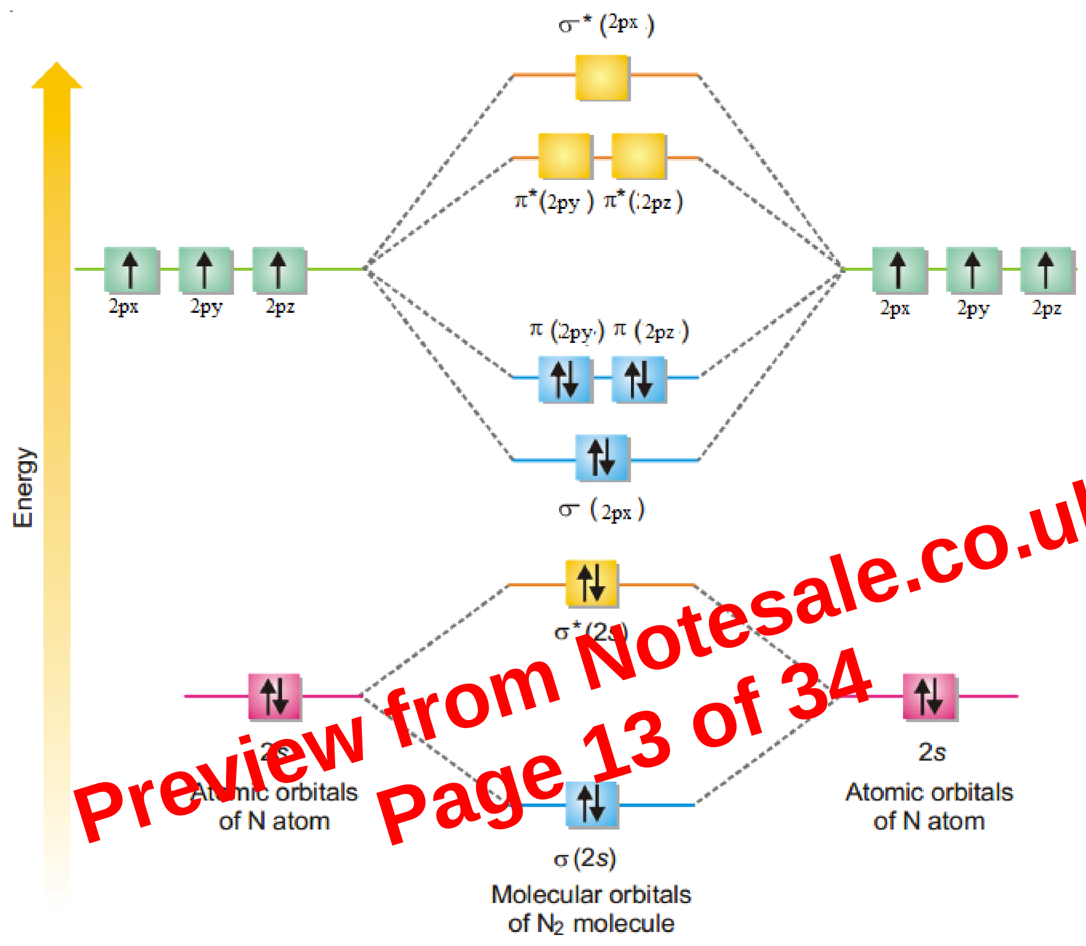


Fig Molecular orbital diagram of N_2 molecule

5. Lithium (Li_2) molecule

Lithium (Li) has electronic configuration $1s^2$, $2s^1$. When two $2s^1$ atomic orbitals of two Li atoms combine to form two molecular orbitals of Li. One is called bonding molecular orbital (σ2s) and the other is called anti bonding molecular orbital (σ*2s). Both the electrons go to the bonding molecular orbital ($\sigma 2s^2$) and the anti-bonding molecular orbital remain vacant ($\sigma^* 2s^0$).

Chemical equation can be represented as;

Bond angle: 180^0

Hybridization: sp

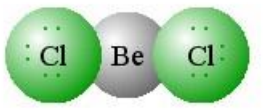
Bond pair: 02

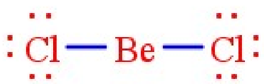
Lone pair: 00

Fig: linear structure of $BeCl_2$

Typical examples of this category are;

$BeCl_2$, $MgCl_2$, $CaCl_2$, $SrCl_2$, $BaCl_2$, BeH_2, MgH_2, CaH_2, SrH_2, BaH_2 etc.

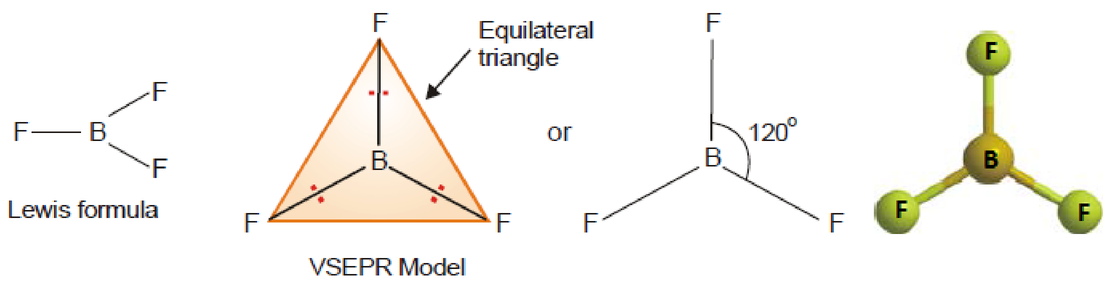


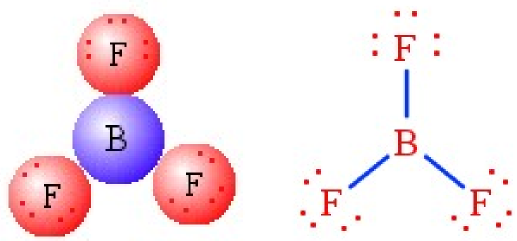


Shapes of molecules containing three electron pairs (AB_3):

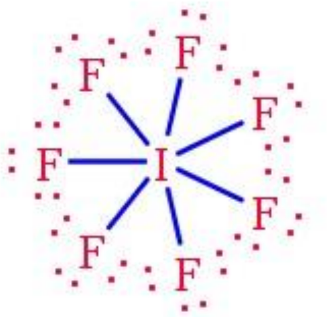
Boron triflouride (BF_3)

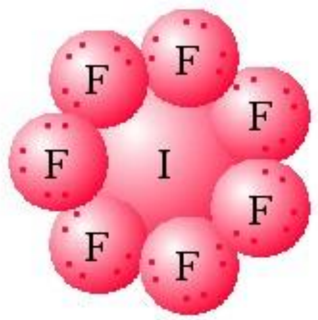
Boron trifluoride has three electrons in valence shell and forming only three covalent bonds. This shows equilateral triangle geometry having bond angle 120^0 and hybridization sp^2. All molecules containing three electrons only and no lone pair will have triangular planar structure.

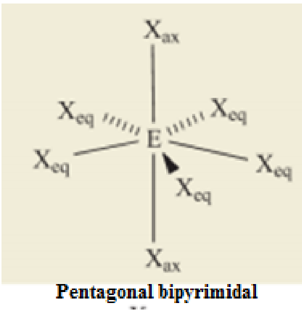




Iodine hexafluoride (IF_7) has seven bond pairs and no lone pairs. Therefore, it has pentagonal bipyrimidal structure having bond angle 72^0 and 90^0. Iodine (I) has seven valence electrons and forms seven covalent bond with fluorine atoms (F). The structure of IF_7 is represented as;







IF_7 IF_7 AB_7

Structure: Pentagonal bipyrimidal

Bond angle: 72^0,90^0

Hybridization: d^3sp^3

Bond pair: 07

Lone pair: 00

Typical examples of this category are;

ClF_7, BrF_7, IF_7.

Shapes of molecules containing bond pairs and lone pairs

Stannous chloride ($SnCl_2$)

Stannous (Sn) has four valence electrons having one bond pair and one lone pair. The lone pair present on Sn pushes the bond pair due to which the bond angle decreases from 120^0 to 116^0. This shows angular structure having bond angle 116^0 and hybridization sp^2.