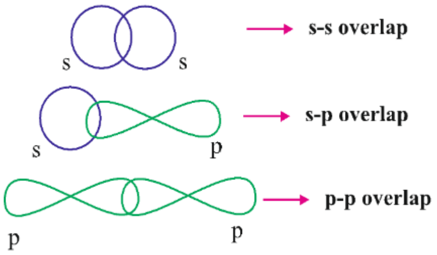
Valance Bond (VB) Theory

- It was first proposed by W. Heitler and F. London in 1927.
- It explains the bonding of atomic orbitals.
- The types of atomic orbitals are s, p, d and f orbitals, each possessing distinct shapes and orientations.
- The overlapping of atomic orbitals results in the formation of a chemical bond and the electrons are localized in the bond region due to overlapping.
- The two main types of overlapping are sigma (σ) and pi (π) bonds, each contributing uniquely to molecular structures. Examples are……



Limitation Valance Bond (VB) Theory

- Failure to explain the tetra-valency exhibited by carbon.
- No insight is offered on the energies of the electrons.
- The theory assumes that electrons are localized in specific areas.
- It does not give a quantitative interpretation of the thermodynamic or kinetic stabilities of coordination compounds.
- No distinction between weak and strong ligands.
- No explanation for the colour exhibited by coordination compounds.

Atomic orbitals

- Each atomic orbital is (designed as s, p, d and f) has unique energy, these varies in shape and spatial orientation eg. 1s, 2s, and 2p orbitals.
- The s orbital is spherical, like a fuzzy hollow ball with its centre of the nucleus of the atom.
- The three p orbitals of equal energy, designated px, py, and pz.
- Each p orbital is dumbbell shaped.

Molecular Orbitals

- Bonding between atom occurs when they come into close enough proximity for their orbitals to overlap. Their electron goes into a single orbital encompassing both nuclei.
- A pair of electrons encompassing two or more nuclei is said to occupy a MOLECULAR ORBITAL
- The molecular orbital represents a lower energy state for the system.

Difference between atomic orbitals and molecular orbitals

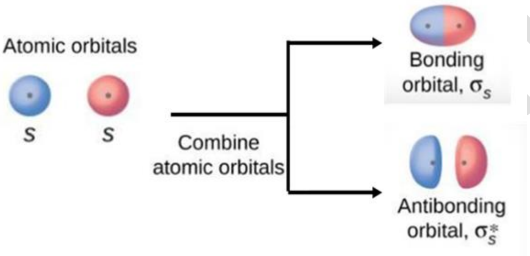
ATOMIC ORBITAL	MOLECULAR ORBITAL
Their electron cloud extends around the nucleus of a single atom i.e. atomic orbital is monocentric	Their electron cloud extends around the nuclei of bonded atoms i.e. molecular orbital is polycentric
They have simple shapes	They have complex shapes
They are represented as s, p, d and f	They are represented by σ, σ*, π, π* etc.

Molecular Orbital Theory

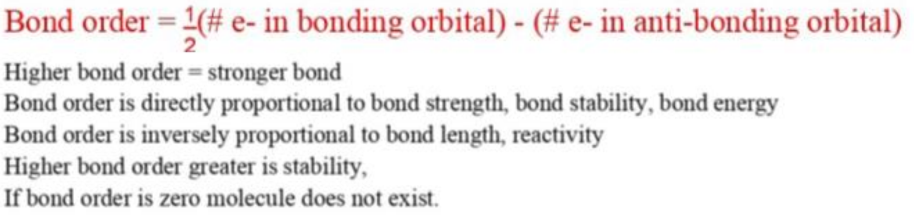
- It was given by Robert S. Mulliken and F. Hunds in 1931.
- It explains nature of covalent bond formation through wave mechanics.
- It explains the characteristic of molecules like their relative bond strength, para and diamagnetic nature.
- According to this theory, atomic orbitals combine and form a resultant orbital known as molecular orbital in which the identity of both atomic orbitals is lost.

The key features of MOT

1. When nuclei of two atoms come close to each other their atomic orbitals interact, to form molecular orbitals in which identity of both atomic orbitals is lost.
2. The total number of molecular orbitals formed will always be equal to the total number of atomic orbitals offered by the bonding species.
3. The electrons in the atomic orbitals are influenced by nucleus, the electron in the molecular orbitals is influenced by all the nuclei.
4. When two atomic orbitals combine, form two new orbitals call bonding and antibonding molecular orbitals.



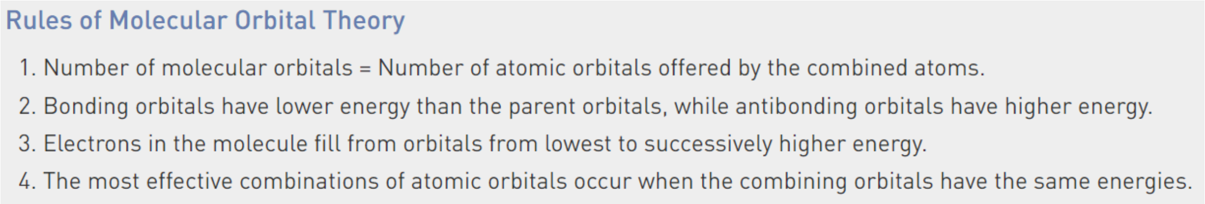
5. The molecular orbital which does not participate in bonding are known as NON-BONDING molecular orbitals. They have essentially the same energy in the molecule as they do in the atomic system.
6. Molecular orbitals are polycentric.
7. Bond order is an indicator of the bond strength and length. A bond order of 1 is equivalent to a single bond. Fractional bond orders are possible.



Bond order = $\frac{1}{2}$(# e- in bonding orbital) - (# e- in anti-bonding orbital)

Higher bond order = stronger bond
Bond order is directly proportional to bond strength, bond stability, bond energy
Bond order is inversely proportional to bond length, reactivity
Higher bond order greater is stability,
If bond order is zero molecule does not exist.

8. The filling of molecular orbitals in a molecule takes place in accordance with Aufbau principle (e- fill the lowest energy MO), Pauli's exclusion principle (first maximum 2e- per orbitals) and Hund's rule (Degenerate orbitals fill singly before they pair).
9. If the MO possess unpaired electrons the molecule is paramagnetic, if the MO have all paired electrons, the molecule is diamagnetic.



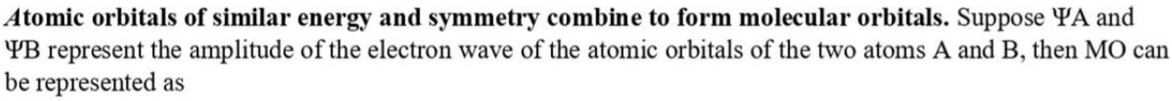
Rules of Molecular Orbital Theory

1. Number of molecular orbitals = Number of atomic orbitals offered by the combined atoms.
2. Bonding orbitals have lower energy than the parent orbitals, while antibonding orbitals have higher energy.
3. Electrons in the molecule fill from orbitals from lowest to successively higher energy.
4. The most effective combinations of atomic orbitals occur when the combining orbitals have the same energies.

Linear combination of atomic orbital (LCAO)

MOT is explained on the basis of LCAO approximation (Electron in atomic orbital is described by wave-function (ψ)

The total number of molecular orbitals formed will always be equal to the total number of atomic orbitals offered by the bonding species.



Atomic orbitals of similar energy and symmetry combine to form molecular orbitals. Suppose ΨA and ΨB represent the amplitude of the electron wave of the atomic orbitals of the two atoms A and B, then MO can be represented as

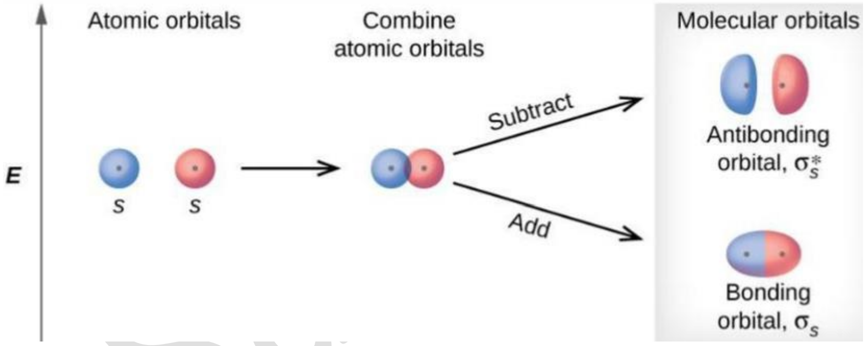
$$\Psi MO = \Psi A \pm \Psi B$$

Molecular orbital formed by addition overlap of wave function ψA and ψB will form **Bonding Molecular Orbital.** It always has lower energy than the energies of combining atomic orbitals and more is the stability.

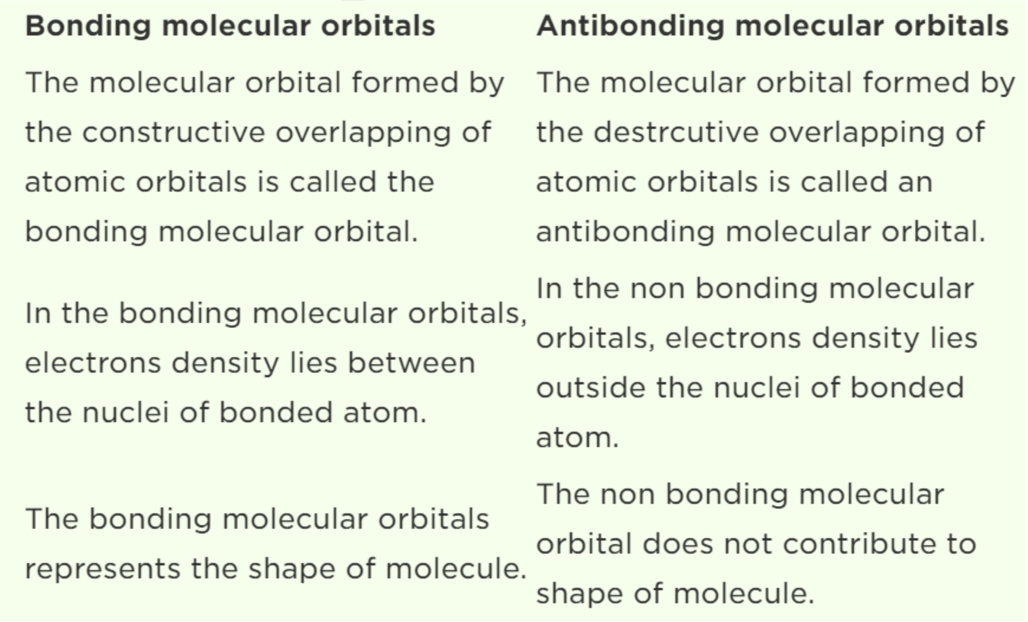
$$\Psi BMO = \Psi A + \Psi B$$

Molecular orbital formed by subtraction overlap of wave function ψA and ψB will form **Antibonding Molecular Orbital.** It always has higher energy than the energies of combining atomic orbitals.

$$\Psi ABMO = \Psi A - \Psi B$$



Difference between bonding and antibonding molecular orbitals

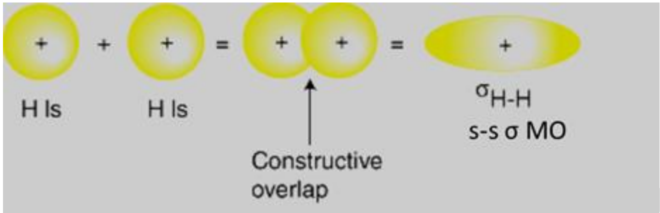


Bonding molecular orbitals	Antibonding molecular orbitals
The molecular orbital formed by the constructive overlapping of atomic orbitals is called the bonding molecular orbital.	The molecular orbital formed by the destrcutive overlapping of atomic orbitals is called an antibonding molecular orbital.
In the bonding molecular orbitals, electrons density lies between the nuclei of bonded atom.	In the non bonding molecular orbitals, electrons density lies outside the nuclei of bonded atom.
The bonding molecular orbitals represents the shape of molecule.	The non bonding molecular orbital does not contribute to shape of molecule.

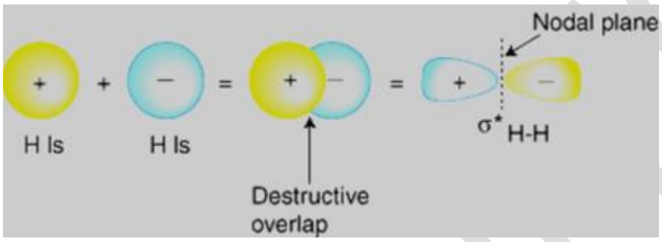
Condition for the combination of atomic orbitals

The atomic orbitals that are involved in the formation of molecular orbitals should have same energy.

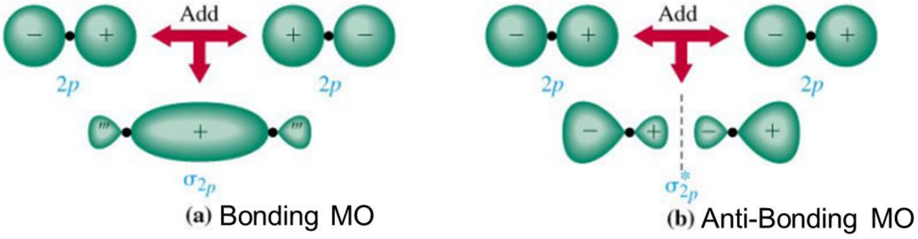
a) Two 1s atomic orbitals (Bonding MO): An s orbital of one atom can be combine with another atom in two ways i.e. additive or subtractive combinations.



Antibonding MO

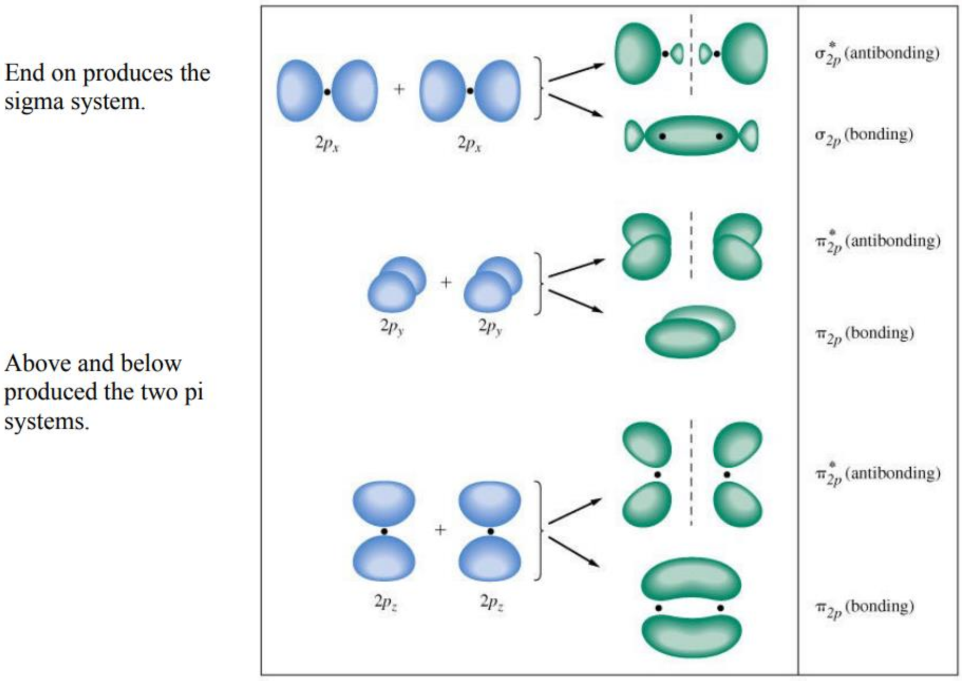


b) Two pz atomic orbitals: Overlap of two p orbitals, which have lobes pointing along the axis joining the nucleus resulting the formation of bonding sigma molecular orbitals and antibonding sigma molecular orbitals.



(a) Bonding MO

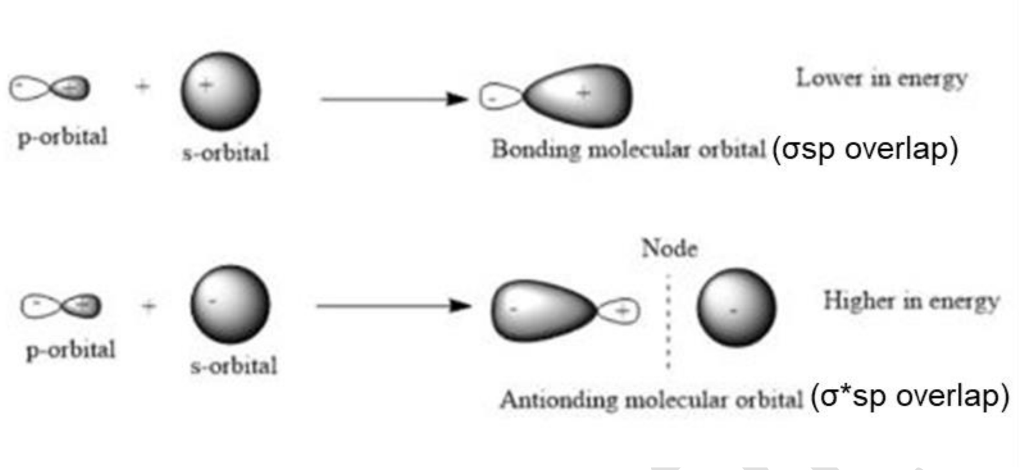
(b) Anti-Bonding MO



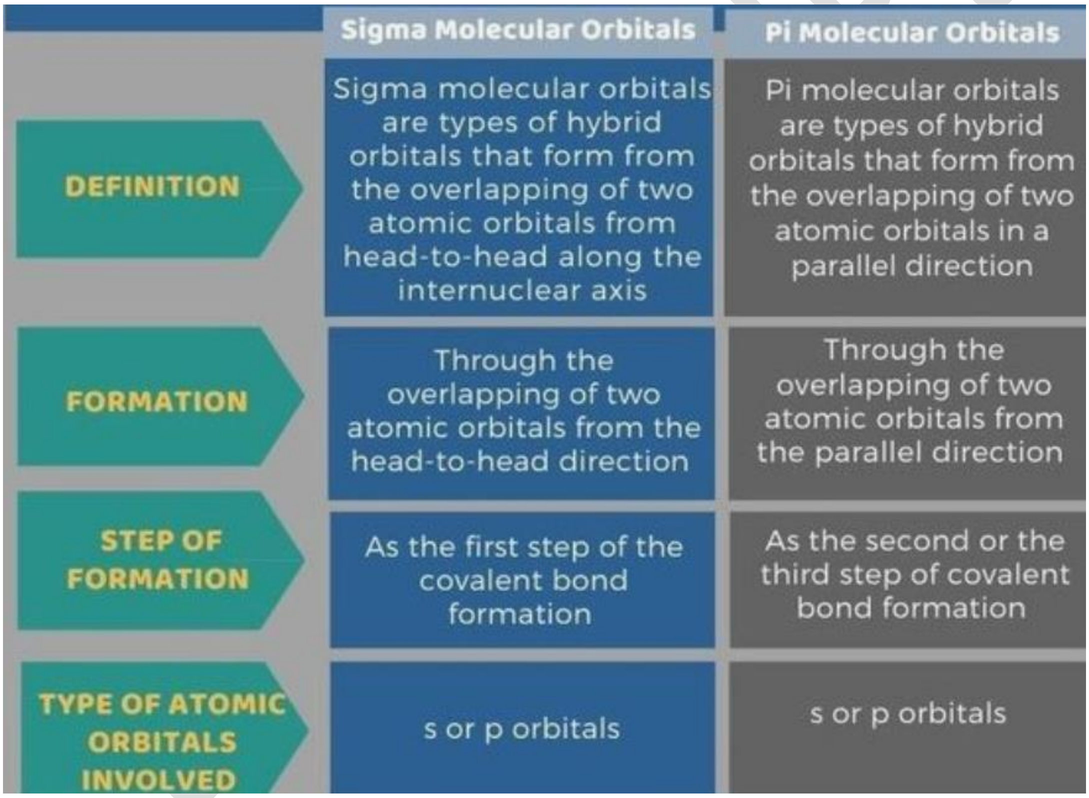
End on produces the sigma system.

Above and below produced the two pi systems.

c) Combination of p and s orbitals: An s orbital combine with p-orbital provided the lobes of p-orbitals are directed along the internuclear axis. When the overlapping lobes have some signs, this gives a bonding molecular orbital.



Difference between sigma and pi molecular orbitals



	Sigma Molecular Orbitals	Pi Molecular Orbitals
DEFINITION	Sigma molecular orbitals are types of hybrid orbitals that form from the overlapping of two atomic orbitals from head-to-head along the internuclear axis	Pi molecular orbitals are types of hybrid orbitals that form from the overlapping of two atomic orbitals in a parallel direction
FORMATION	Through the overlapping of two atomic orbitals from the head-to-head direction	Through the overlapping of two atomic orbitals from the parallel direction
STEP OF FORMATION	As the first step of the covalent bond formation	As the second or the third step of covalent bond formation
TYPE OF ATOMIC ORBITALS INVOLVED	s or p orbitals	s or p orbitals

Energy level diagram for molecular orbitals

The energy level diagram for homonuclear molecule (B_2, C_2, N_2) is:

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

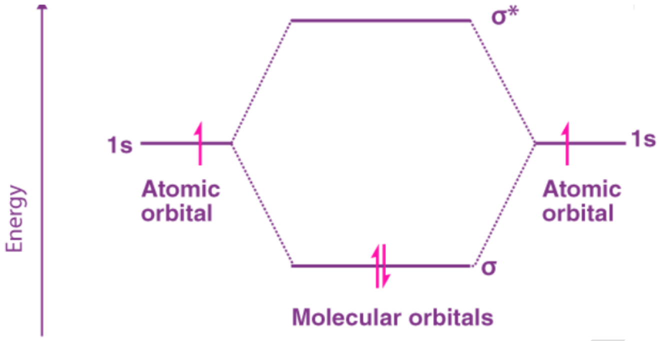
The energy level diagram for homonuclear molecule (O_2, F_2, Ne_2) is:

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

The bonding π2px and π2py MO's have exactly the same energy and are said to be double degenerative.

Draw molecular orbital diagram of H_2 molecule. Calculate its bond order and find its magnetic nature.

The electronic configuration of H_2 is $\sigma(1s^2)$.



No. of bonding orbitals (N_b)= 2, No. of antibonding orbitals $N_a = 0$

∴ Bond order = 1, the molecule is stable since it is a positive value.

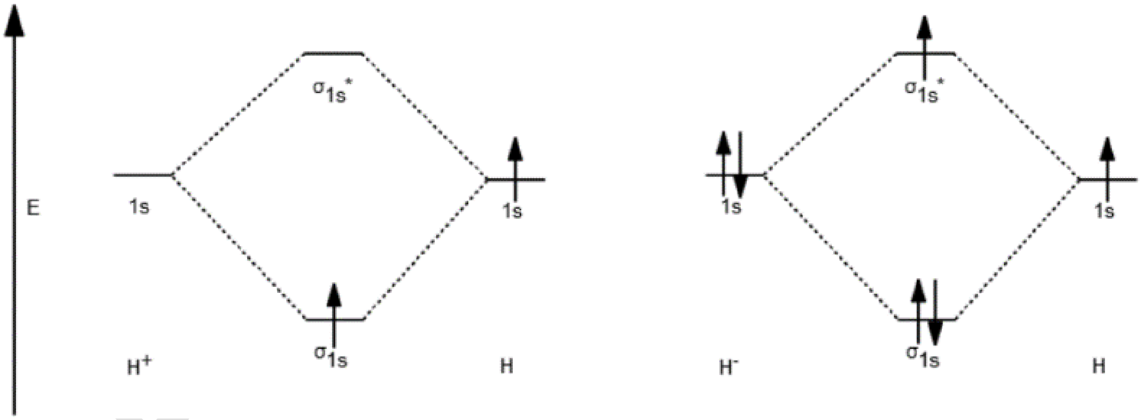
The two hydrogen atoms are connected by a single bond.

Since there are no unpaired electrons, the H_2 molecule is diamagnetic.

Compare with H_2^+ and H_2^-

Each hydrogen atom contributes one electron, and thus, **H_2^-** has three electrons while **H_2^+** has one electron.

Each hydrogen atom contributes one 1s atomic orbital, and thus, the orbitals overlap according to MO theory to form one σ1s and one σ*1s MO by conservation of orbitals.



Bond order for **H_2^+**

$$\frac{No.of\ Bonding\ electrons - No.of\ Antibonding\ electrons}{2} = \frac{1-0}{2} = 0.5$$

Bond order for **H_2^-**

$$\frac{No.of\ Bonding\ electrons - No.of\ Antibonding\ electrons}{2} = \frac{2-1}{2} = 0.5$$

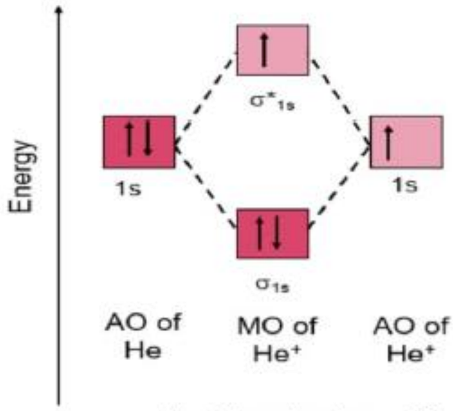
Both have one unpair electron thus they show paramagnetic nature. So, neither is more stable than the other. But of course, they are less stable than H_2.

Compare He_2 and He_2^+

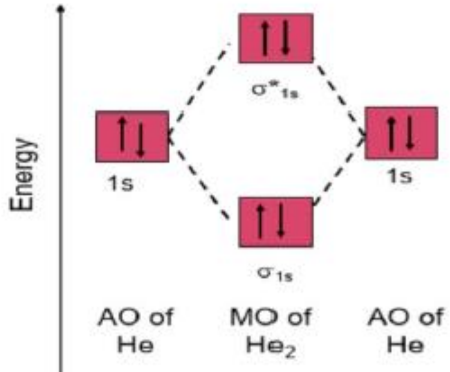
Each He atoms have 2 electrons, its configuration is $1s^2$

It has 4 electrons and molecular orbital configuration is $\sigma 1s^2, \sigma^* 1s^2$

While MO configuration for He_2^+ is $\sigma 1s^2, \sigma^* 1s^1$



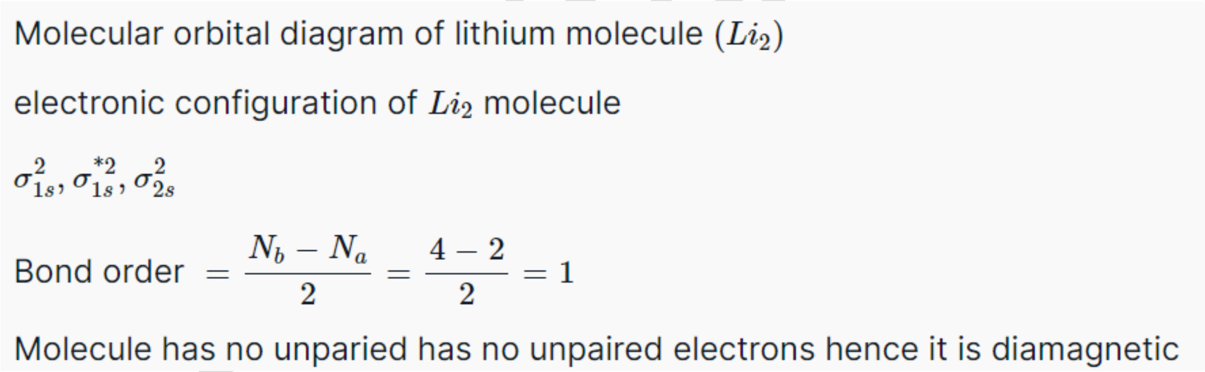
He_2^+ bond order = 1/2



He_2 bond order = 0

Number of electrons in He_2 = 2 [B.O.= 2-2/2= 0]
Number of electrons in He_2^+= 3 [B.O.= 2-1/2= 0.5]

Hence bond order of He_2 is zero hence, He_2 is not exist.



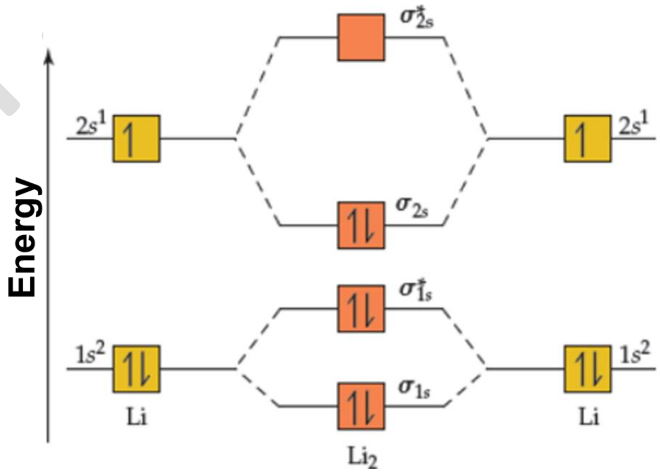
Molecular orbital diagram of lithium molecule (Li_2)

electronic configuration of Li_2 molecule

$\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2$

Bond order $= \dfrac{N_b - N_a}{2} = \dfrac{4-2}{2} = 1$

Molecule has no unparied has no unpaired electrons hence it is diamagnetic



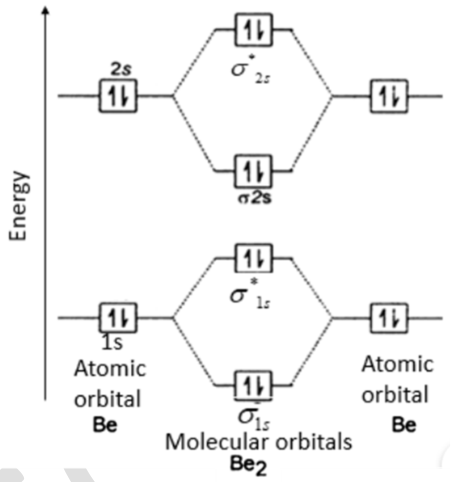
Be_2

Be has four electrons, hence Be_2 molecule has 8 electrons. Its configuration is $\sigma 1s^2$, $\sigma^* 1s^1$, $\sigma 2s^2$, $\sigma^* 2s^2$

Here $N_b = 2$, $N_a = 2$

Bond order $= \frac{1}{2}[N_b - N_a] = \frac{1}{2}[2-2] = 0$

Magnetic property: Since bond order is zero, Be_2 molecule does not exist. It is diamagnetic due to the absence of any unpaired electron.



Boron (B_2)

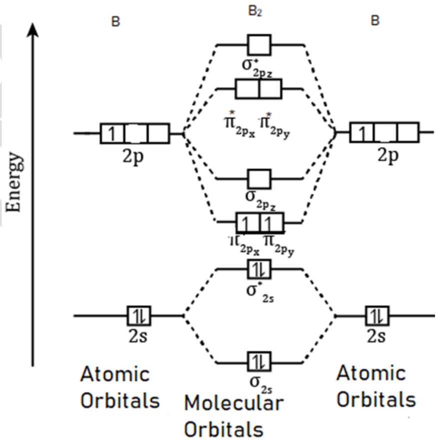
Boron (B) has five electrons, when two atoms of boron combines to form B_2 molecule it contains 10 electrons. Its configuration of B_2 is $\sigma 1s^2$, $\sigma^* 1s^1$, $\sigma 2s^2$, $\sigma^* 2s^2$ $\pi 2p_x^1 = \pi 2p_y^1$

Bond order: Here Nb = 4, Na = 2

Bond order = Bond order $= \frac{1}{2}[N_b - N_a] = \frac{1}{2}[4-2] = 1$

The two boron atom is B2 molecules are linked by one covalent bond.

Magnetic properties: Since each $\pi 2p_x$ and $\pi 2p_y$ MO contains unpaired electron, therefore B_2 molecule is paramagnetic.



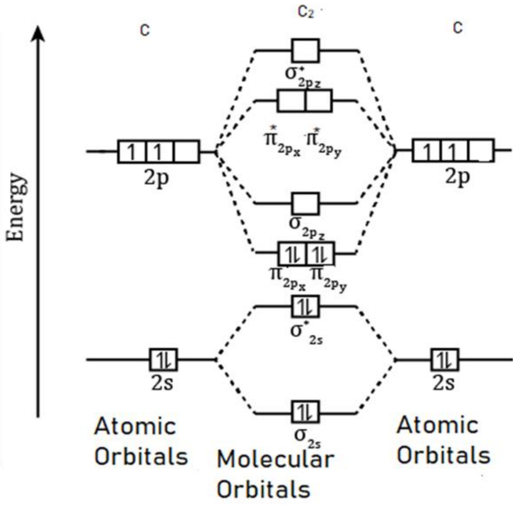
Carbon (C_2)

- Electronic configuration of Carbon (C) is $1s^2\ 2s^2 2p^2$.
- Total number of electrons in C_2 molecule is 6 + 6 =12
- The molecular orbital electronic configuration of C_2 is

$$\left[\sigma\ (1s)^2\right] \left[\sigma^*(1s)^2\right] \left[\sigma(2s)^2\right] \left[\sigma^*(2s)^2\right] \left[\pi(2px)^2\right] \left[\pi\ (2py)^2\right]$$

- Number of electrons in bonding orbital = 8
- Number of electrons in anti-bonding orbital = 4
- Therefore, bond order = $\frac{1}{2}(8-4) = 2$
- Hence, the bond order of the C_2 molecule is 2 and it will have a double bond.

C_2 is a stable molecule. All the electrons are paired in molecular orbital. Its diamagnetic in nature.



N_2 molecule

Two nitrogen atoms overlap to form N_2 molecule and total 14 electrons are filled in MO of N_2

Electronic configuration:

$$\sigma 1s^2 < \sigma^* 1s^2 < \sigma 2s^2 < \sigma^* 2s^2 , [\pi 2p_x^2 = \pi 2p_y^2] < \sigma 2p_z^2 < [\pi^* 2p_x = \pi^* 2p_y] < \sigma^* 2p_z$$

Let's calculate the bond order of N_2:

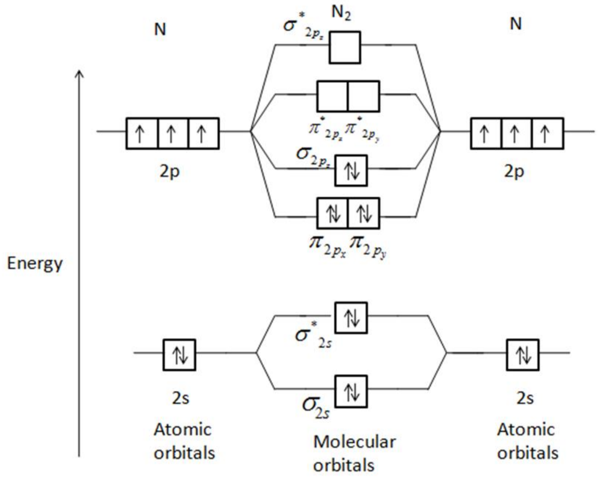
$$\text{Bond order} = \frac{\text{Bonding electrons} - \text{Anti bonding electrons}}{2}$$

$$= \frac{10-4}{2} = 3$$

Therefore, the order of N_2 is 3.

: N≡N :

N_2 does not have unpaired electrons, hence it is diamagnetic.



Draw the molecular orbital diagram of N_2, N_2^+, N_2^-, N_2^{2-}. Write their electronic configuration, find the bond order and predict their magnetic behavior. Arrange the above in increasing order of bond length.

Atomic number of nitrogen is seven. Therefore in N_2 there are a total fourteen electrons. But N_2^+ has one electron less than that of nitrogen molecules. So, total electrons are thirteen. Molecular orbital diagram of N_2^+ is shown below:

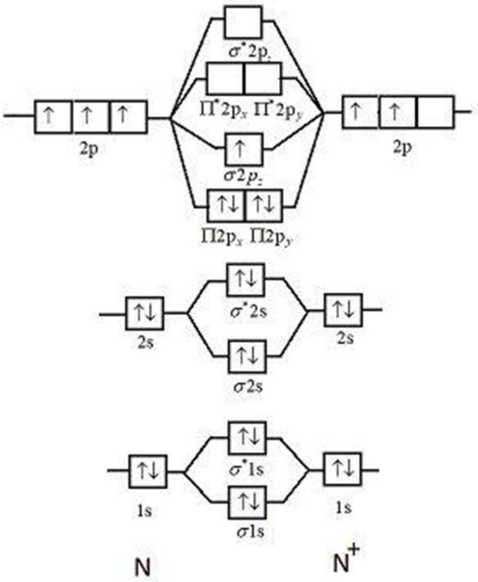
Electronic configuration of N_2^+ is:

$$(\sigma 1s)^2(\sigma^* 1s)^2(\sigma 2s)^2(\sigma^* 2s)^2(\Pi 2p_x)^2(\Pi 2p_y)^2\ (\sigma 2p_z)$$

$$\text{Bond order} = \frac{9-4}{2}$$

$$\text{Bond order} = 2.5$$

From the diagram we can see that in N_2^+ only one electron is unpaired. Hence it is magnetic in nature .



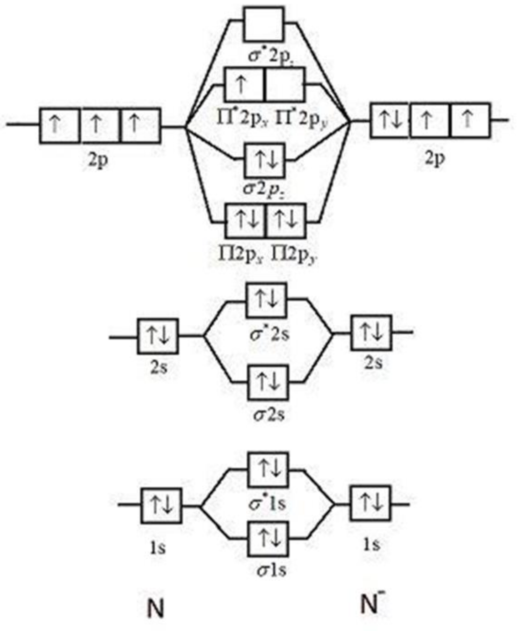
In case of N_2^- has one electron more than that of nitrogen molecule. So, total electrons are fifteen.

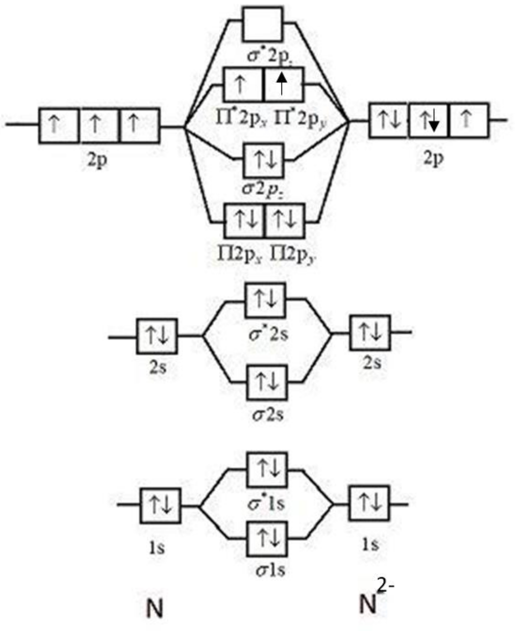
Electronic configuration of N_2^- is:

$$(\sigma 1s)^2(\sigma^* 1s)^2(\sigma 2s)^2(\sigma^* 2s)^2(\Pi 2p_x)^2(\Pi 2p_y)^2(\sigma 2p_z)^2\ (\Pi^* 2p_x)$$

$$\text{Bond order} = \frac{10-5}{2}$$

$\text{Bond order} = 2.5$ From the diagram we can see that in N_2^- only one electron is unpaired. Hence it is magnetic in nature.





In case of N_2^{-2} has one electron more than that of nitrogen molecule. So, total electrons are fifteen.

$$(\sigma 1s)^2(\sigma^* 1s)^2(\sigma 2s)^2(\sigma^* 2s)^2(\Pi 2p_x)^2(\Pi 2p_y)^2(\sigma 2p_z)^2\ (\Pi^* 2p_x)^1(\Pi^* 2p_y)^1$$

$$\text{Bond order} = \frac{10-6}{2}$$

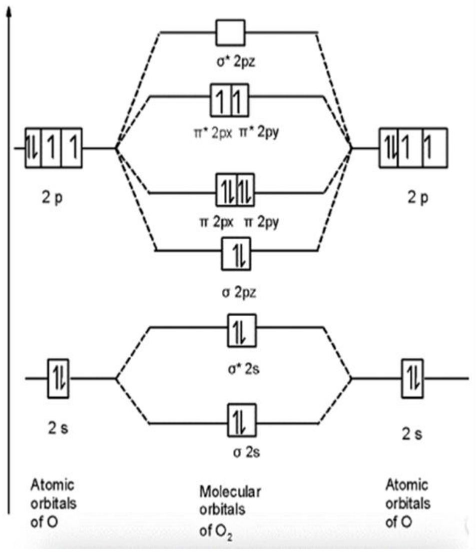
$$\text{Bond order} = 2$$

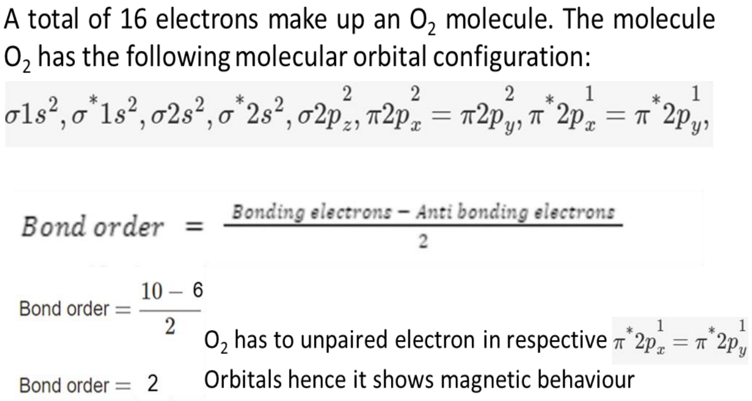
From the diagram we can see that in N_2^{-2} only one electron is unpaired. Hence it is magnetic in nature.

N_2> N_2^+ = N_2^-, N_2^{2-} Stability order for the series.

O_2 molecule

Oxygen molecule has 16 electrons, so the electronic configuration of oxygen molecule becomes:





A total of 16 electrons make up an O_2 molecule. The molecule O_2 has the following molecular orbital configuration:

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

$$\text{Bond order} = \frac{\text{Bonding electrons} - \text{Anti bonding electrons}}{2}$$

$$\text{Bond order} = \frac{10-6}{2}$$

$$\text{Bond order} = 2$$

O_2 has to unpaired electron in respective $\pi^* 2p_x^1 = \pi^* 2p_y^1$ Orbitals hence it shows magnetic behaviour

For the species O_2, O_2^+, and O_2^-, give the electron configuration and the bond order for each. Which has the strongest bond?

The O_2 molecule has 12 valence electrons (6 + 6); O_2^+ has 11 valence electrons (6 + 6 − 1); and O_2^- has 13 valence electrons (6 + 6 + 1). We will assume that the ions can be treated using the same molecular orbital diagram as for the neutral diatomic molecule:

	O_2	O_2^+	O_2^-	O_2^{2-}
σ_{2p}^*	—	—	—	—
π_{2p}^*	↑ ↑	↑ –	⇅ ↑	⇅ ⇅
π_{2p}	⇅ ⇅	⇅ ⇅	⇅ ⇅	⇅ ⇅
σ_{2p}	⇅	⇅	⇅	⇅
σ_{2s}^*	⇅	⇅	⇅	⇅
σ_{2s}	⇅	⇅	⇅	⇅

The electron configuration for each species can then be taken from the diagram:

O_2: $(\sigma_{2s})^2(\sigma_{2s}^*)^2(\sigma_{2p})^2(\pi_{2p})^4(\pi_{2p}^*)^2$

O_2^+: $(\sigma_{2s})^2(\sigma_{2s}^*)^2(\sigma_{2p})^2(\pi_{2p})^4(\pi_{2p}^*)^1$

O_2^-: $(\sigma_{2s})^2(\sigma_{2s}^*)^2(\sigma_{2p})^2(\pi_{2p})^4(\pi_{2p}^*)^3$

O_2^{2-}: $(\sigma_{2s})^2(\sigma_{2s}^*)^2(\sigma_{2p})^2(\pi_{2p})^4(\pi_{2p}^*)^4$

The bond orders are:

For O_2: $\frac{10-6}{2} = 2$ Paramagnetic

For O_2^+: $\frac{8-3}{2} = 2.5$ Paramagnetic

For O_2^-: $\frac{10-7}{2} = 1.5$ Paramagnetic

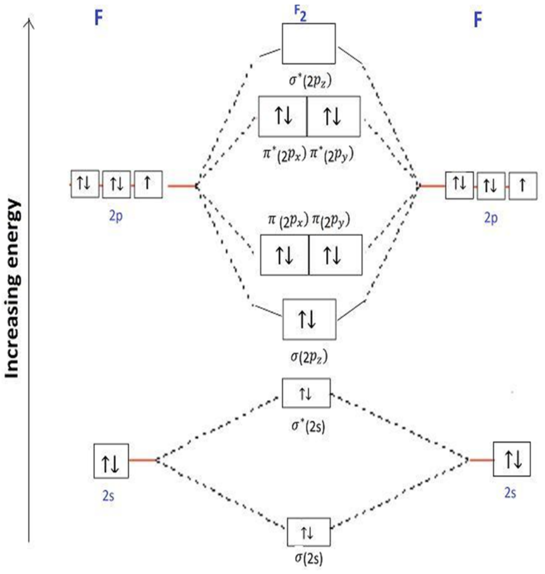
For O_2^{2-}: $\frac{10-8}{2} = 1$ Diamagnetic

Thus, O_2^+ is expected to have the strongest bond

Stability ∝ B.O

∴ Stability order $[O_2^+ > O_2 > O_2^- > O_2^{2-}]$

F_2 molecule



$F_2(18) =$

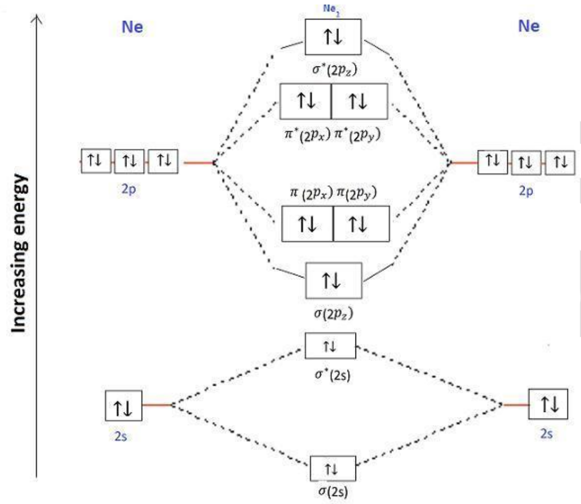
$\sigma 1s^2\ \sigma*1s^2\ \sigma 2s^2\sigma*2s^2\ \sigma 2s^2\sigma*2s^2\sigma 2p_z^2\pi 2p_x^2 = \pi 2p_y^2\pi^*2p_x^2 = \pi^*2p_y^2$

Bond Order $(N_2) = \frac{1}{2}(10-4) = 3$

So, the bond order is 3. hence, it would have a triple bond.

Molecule is diamagnetic in nature

Neon (Ne_2)



$Ne_2(20):$

$Ne_2(20): \sigma 1s^2\ \sigma s^2\ \sigma 2s^2\sigma*2s^2\sigma 2p_z^2\pi 2p_x^2 = \pi 2p_y^2\pi^*2p_x^2 = \pi^*2p_y^2\ \sigma^*2p_z^2$

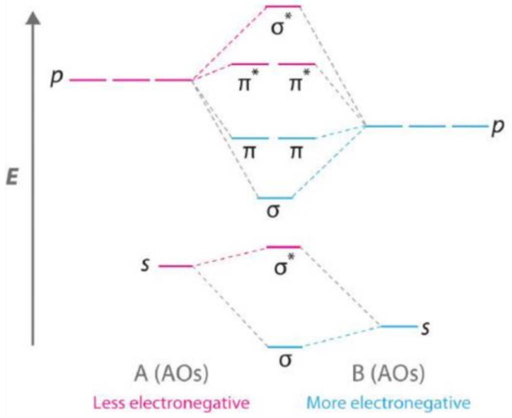
Bond Order $(Ne_2) = \frac{1}{2}(10-10) = 0$

No bond formed in Ne_2 molecule. So, Ne_2 molecule would not exist.

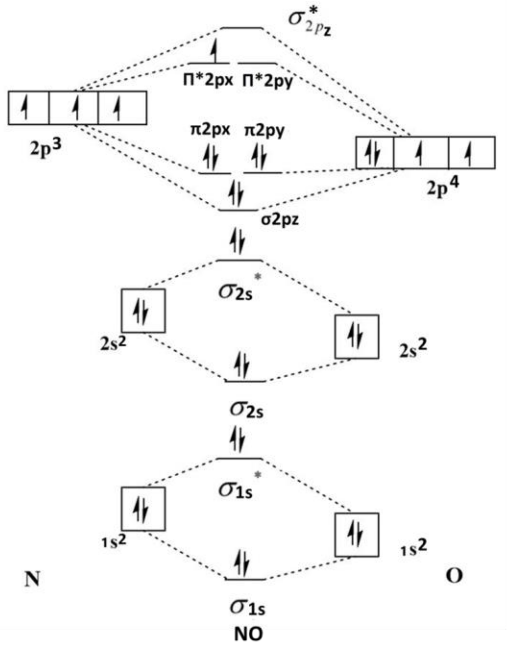
MO diagrams for Heteronuclear Diatomic Molecules

Similar approach follows to making MO diagram for heteronuclear di-atomic molecules. Two major rules were follows:

1. More electron negative atom fills their electron in bonding orbital (having low energy), while less electronegative atom fills their electrons in anti-bonding orbitals (high energy).
2. More electron negative atom placed on the right hand side of the MO diagram whereas, less electron negative atom placed at the left side.



Nitric Oxide (NO)



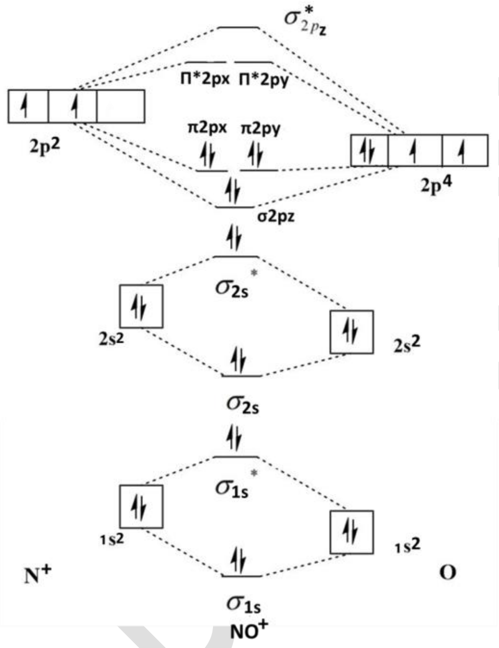
N has an atomic number of 7 and O has an atomic number of 8. There will be a total of 15 electrons. The electronic configuration of NO is

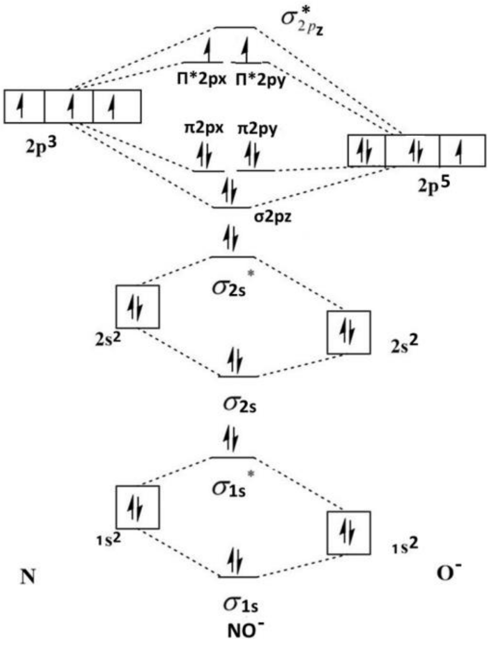
$$\sigma\left(1s^2\right)\sigma^*\left(1s^2\right)\sigma\left(2s^2\right)\sigma^*\left(2s^2\right)\sigma(2p_z)^2\,\pi(2p_x)^2\,\pi(2p_y)^2\,\pi^*(2p_x)^1$$

. Bond order = $\frac{N_b-N_a}{2}$ = $\frac{10-5}{2}$ = 2.5

Molecule is paramagnetic nature due to the presence of unpaired electrons

NO$^+$ and NO$^-$ molecules





For NO$^+$

N has an atomic number of 6 and O has an atomic number of 8. There will be a total of 14 electrons. The electronic configuration of NO$^+$ is

$$\sigma\left(1s^2\right)\sigma^*\left(1s^2\right)\sigma\left(2s^2\right)\sigma^*\left(2s^2\right)\sigma(2p_z)^2\,\pi(2p_x)^2\,\pi(2p_y)^2\,\pi^*(2p_x)$$

Bond order = $\frac{N_b-N_a}{2}$ = $\frac{10-4}{2}$ = 3

Molecule is diamagnetic nature due to the absence of unpaired electrons

For NO$^-$

N has an atomic number of 7 and O has an atomic number of 9. There will be a total of 16 electrons. The electronic configuration of NO$^-$ is

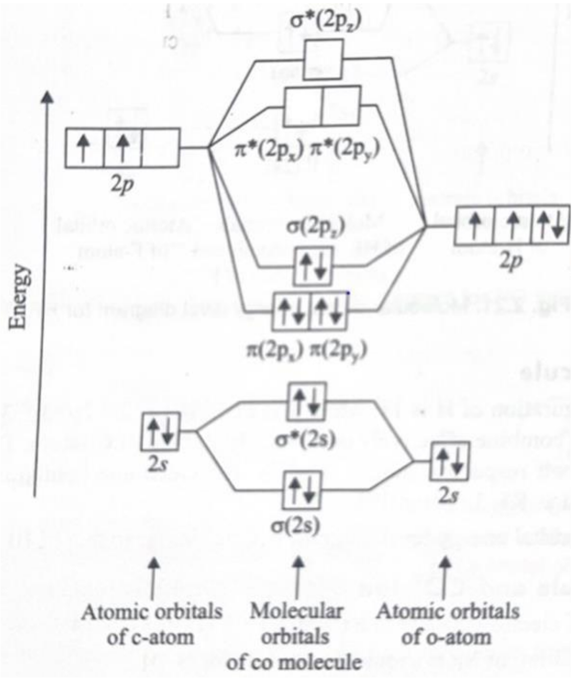
$$\sigma\left(1s^2\right)\sigma^*\left(1s^2\right)\sigma\left(2s^2\right)\sigma^*\left(2s^2\right)\sigma(2p_z)^2\,\pi(2p_x)^2\,\pi(2p_y)^2\,\pi^*(2p_x)^1(\Pi^*2p_y)^1$$

. Bond order = $\frac{N_b-N_a}{2}$ = $\frac{10-6}{2}$ = 2

Molecule is paramagnetic nature due to the presence of Two unpaired electrons

Stability NO$^+$ > NO > NO$^-$

CO Molecule



C has an atomic number of 6 and O has an atomic number of 8. There will be a total of 14 electrons. The electronic configuration of NO is

$$\sigma\left(1s^2\right)\sigma^*\left(1s^2\right)\sigma\left(2s^2\right)\sigma^*\left(2s^2\right)\pi(2p_x)^2\pi(2p_y)^2\sigma(2p_z)^2$$

Bond order = $\frac{N_b - N_a}{2} = \frac{10-4}{2} = 3$

Molecule is diamagnetic nature due to the absence of unpaired electrons

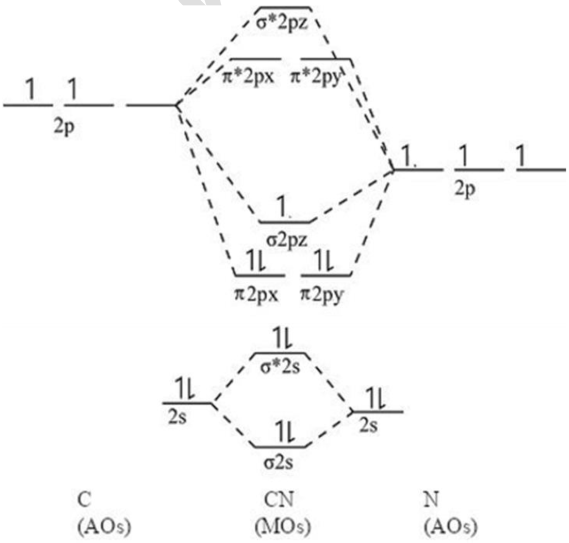
For CO+

C has an atomic number of 6 and O has an atomic number of 8. In case CO+, one electron loses from C atom due to its less negative nature. There will be a total of 13 electrons. The electronic configuration of CO+ is

$$\sigma\left(1s^2\right)\sigma^*\left(1s^2\right)\sigma\left(2s^2\right)\sigma^*\left(2s^2\right)\pi(2p_x)^2\pi(2p_y)^2\sigma(2p_z)^1$$

Bond order = $\frac{N_b - N_a}{2} = \frac{9-4}{2} = 2.5$ Molecule is paramagnetic nature due to the presence of one unpaired electron.

CN molecule



The number of electrons in carbon is 6 and the number of electrons in nitrogen is 7.

- Therefore the CN molecule contains 13 electrons.
- The molecular electronic configuration of CN molecules is as follows.

$$\sigma\left(1s^2\right)\sigma^*\left(1s^2\right)\sigma\left(2s^2\right)\sigma^*\left(2s^2\right)\pi(2p_x)^2\pi(2p_y)^2\sigma(2p_z)^1$$

Bond order = $\frac{N_b - N_a}{2} = \frac{9-4}{2} = 2.5$

Molecule is paramagnetic nature due to the presence of one unpaired electrons

For CN$^-$

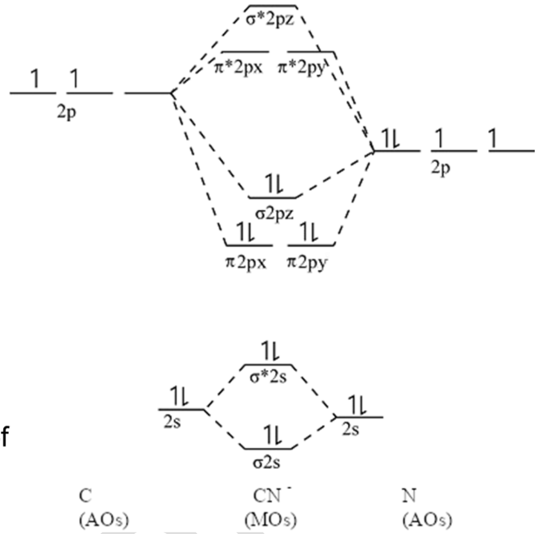
The number of electrons in carbon is 6 and the number of electrons in nitrogen is 7.

- In case of CN$^-$ molecule 13 electrons are present
- The molecular electronic configuration of CN$^-$ molecules is as follows.

$$\sigma\left(1s^2\right)\sigma^*\left(1s^2\right)\sigma\left(2s^2\right)\sigma^*\left(2s^2\right)\pi(2p_x)^2\pi(2p_y)^2\sigma(2p_z)^2$$

Bond order = $\frac{N_b - N_a}{2} = \frac{10-4}{2} = 3$

Molecule is diamagnetic nature due to the absence of unpaired electrons



HF molecule

H has an atomic number of 1 and F has an atomic number of 9. There will be a total of 10 electrons. The electronic configuration of HF is
$1s^2\ 2s^2\ \sigma^2 sp_z\ 2px^2 = 2py^2$

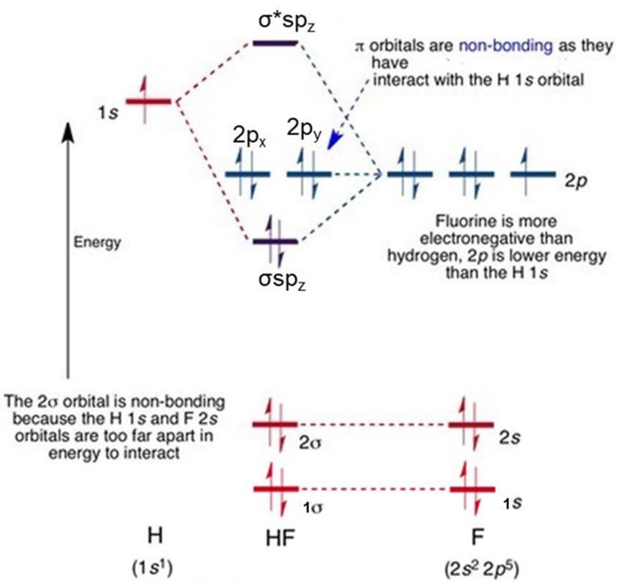
In this case, the energy level of 1s and 2s orbital of fluorine (40.2 eV) is much lower than the energy level of 1 s of hydrogen atom (-13.6eV) therefore it leads the interaction between the 1s orbital of hydrogen and the 2p orbital of fluorine

Due to almost similar energies of the orbitals allowing them to form sigma-bonding and a sigma-antibonding molecular orbital.

The 2px and 2py orbitals of fluorine remain non bonding, each with a pair of electrons.

Bond order = $\frac{N_b - N_a}{2} = \frac{2-0}{2} = 1$

Molecule is diamagnetic nature due to the absence of unpaired electrons



HCl molecule

H has an atomic number of 1 and Cl has an atomic number of 17. There will be a total of 18 electrons. The electronic configuration of HF is
$1s^2\ 2s^2\ 2p6\ 3s2\ \sigma^2 sp_z\ 3px^2 = 3py^2$

In this case, due to the similar energy level of 1 s of hydrogen atom and 3p orbitals of chlorine atom leads formation of sigma-bonding and a sigma-antibonding molecular orbital.

The 1s, 2s, 2p, 3s and 3px and 3py orbitals of fluorine remain non bonding, each with a pair of electrons.

Bond order = $\frac{N_b - N_a}{2} = \frac{2-0}{2} = 1$

Molecule is diamagnetic nature due to the absence of unpaired electrons