

CHEMICAL BONDING - II

PART II

❖ **By:**

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Principal

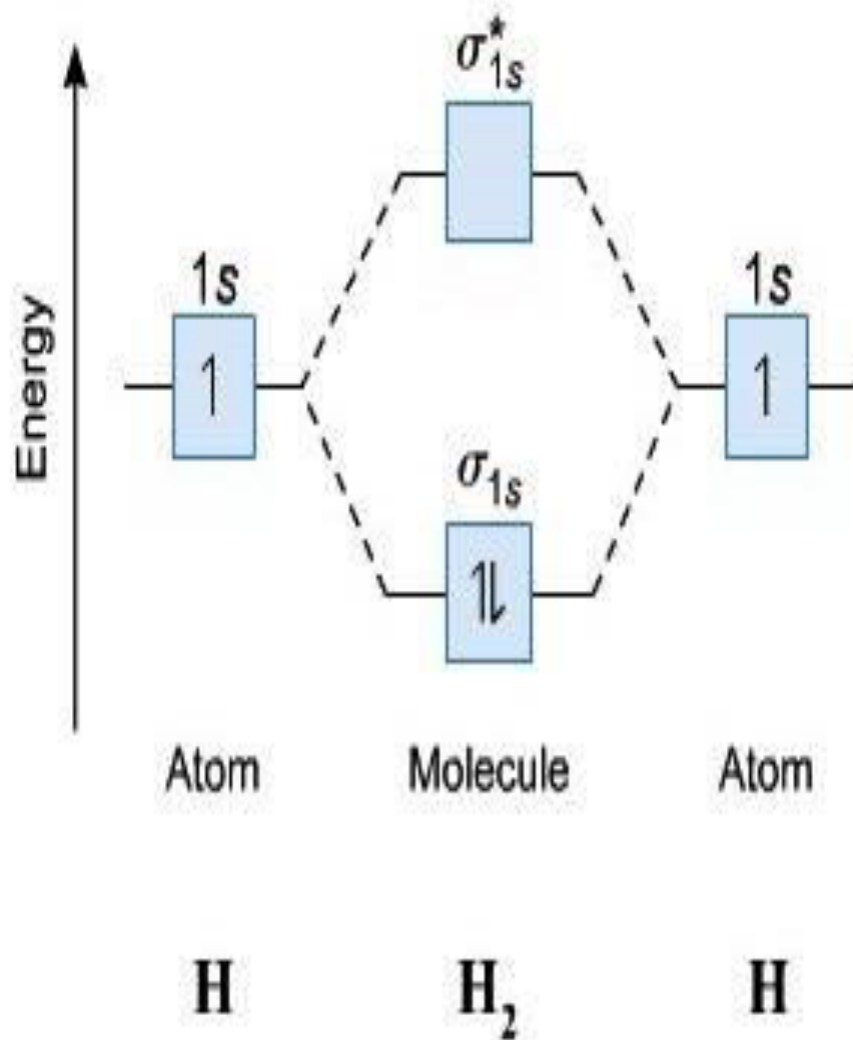
Government Shivalik College,

Naya Nangal

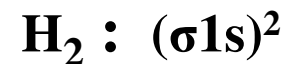
BONDING IN HOMONUCLEAR DIATOMIC MOLECULES

1. HYDROGEN MOLECULE (H₂)

- It is formed by combination of two hydrogen atoms.
- The electronic configuration of each hydrogen atom is **1s¹**.
- Both the hydrogen atoms contribute two electrons towards bond formation.
- Both the electrons are placed in the bonding molecular orbital, **σ1s**.
- The two electrons should have opposite spins according to Pauli's exclusion principle.



- The molecular orbital electronic configuration of H₂ molecule is :



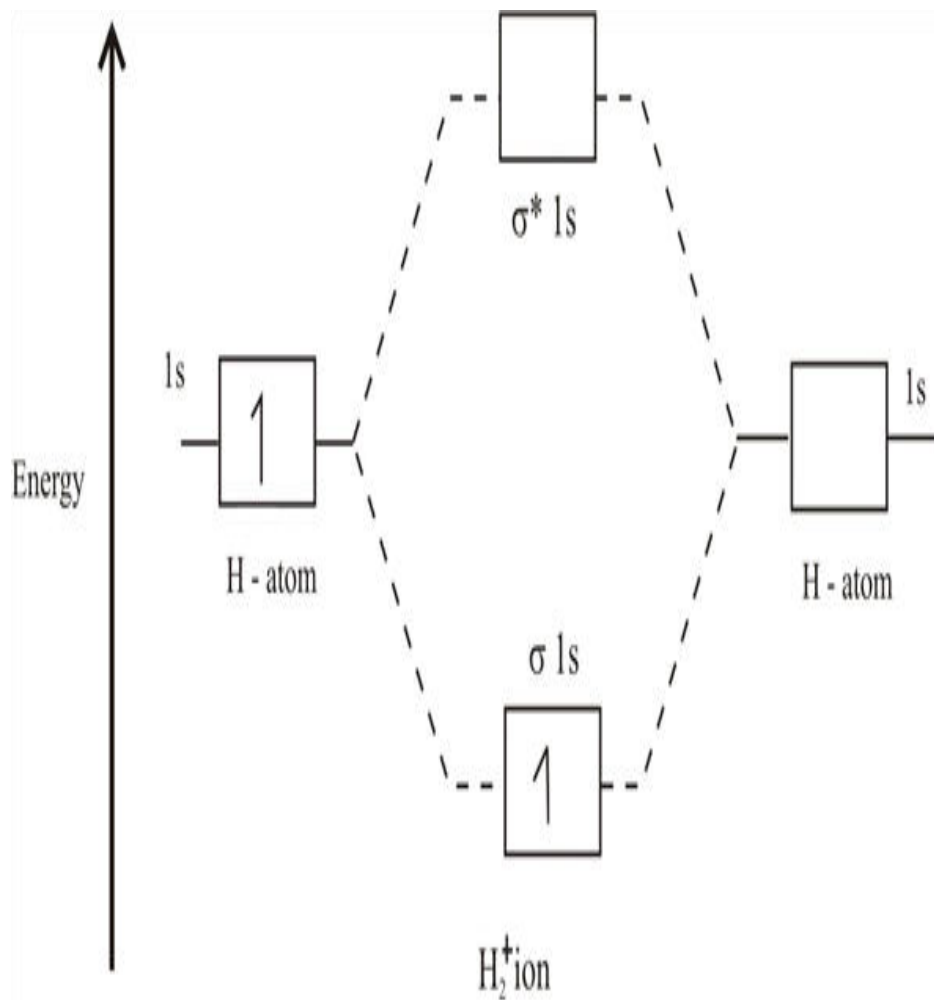
- The bond order is

$$\begin{aligned} \text{Bond order} &= \frac{N_b - N_a}{2} \\ &= \frac{2 - 0}{2} = 1 \end{aligned}$$

- The two hydrogen atoms are bonded by a single covalent bond.
- B. D. Energy = 458 kJ/mol
- Bond length = 0.74 Å
- Diamagnetic in nature

2. HYDROGEN MOLECULE (H_2^+) ION

- Hydrogen molecular ion has no real existence.
- It is the simplest molecule ion that has been spectroscopically discovered when an electric discharge is passed through hydrogen gas under reduced pressure.
- It is formed by the combination of hydrogen atom having electronic configuration $1s^1$ and a hydrogen ion having electronic configuration $1s^0$
- The molecule has only one electron which is placed in $\sigma 1s$ bonding MO.



Energy level diagram

- The molecular orbital electronic configuration of H_2^+ molecule is :

$$\text{H}_2^+ : (\sigma 1s)^1$$

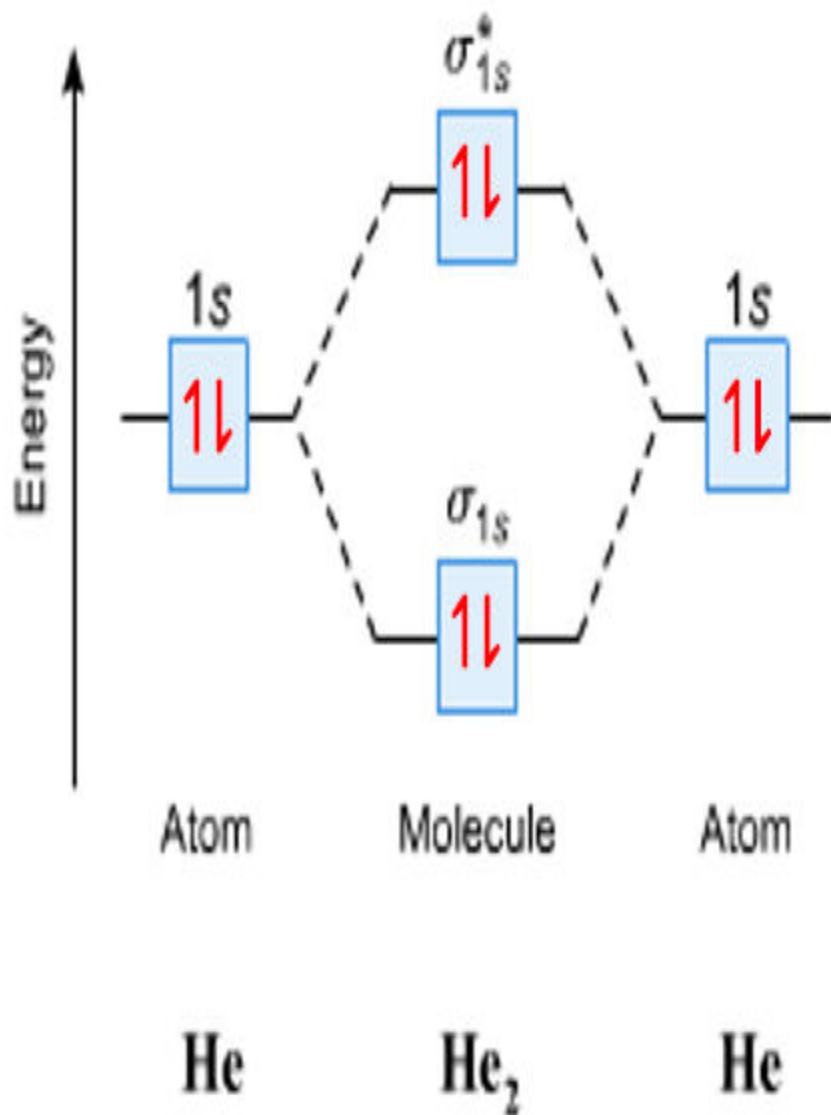
- The bond order is

$$\begin{aligned} \text{Bond order} &= \frac{N_b - N_a}{2} \\ &= \frac{1 - 0}{2} = \frac{1}{2} \end{aligned}$$

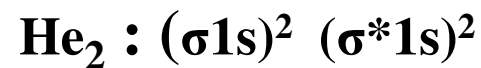
- The bond length of H_2^+ ion is **larger** than H_2 molecule while its bond dissociation is **less** than H_2 molecule
- B. D. Energy = 255 kJ/mol
- Bond length = 1.06 Å
- Paramagnetic in nature

3. *HYPOTHETICAL HELIUM MOLECULE (He₂)*

- It is formed by combination of two helium atoms.
- The electronic configuration of each helium atom is $1s^2$.
- Both the helium atoms contribute four electrons towards bond formation.
- Two of the four electrons are placed in the bonding molecular orbital, $\sigma 1s$ whereas the remaining two are placed in the antibonding molecular orbital $\sigma^* 1s$.
- The electrons should have opposite spins according to Pauli's exclusion principle.



- The molecular orbital electronic configuration of **He₂** molecule is :



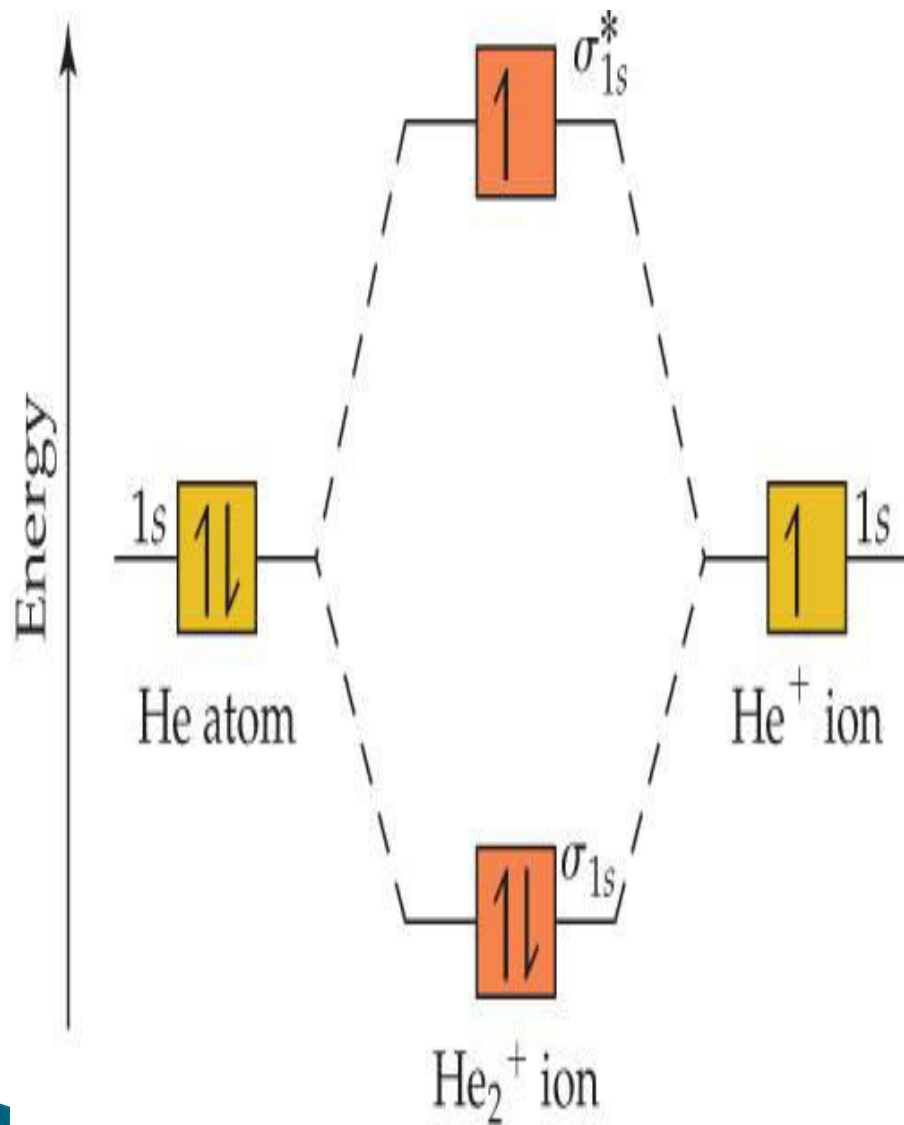
- The bond order is

$$\begin{aligned} \text{Bond order} &= \frac{N_b - N_a}{2} \\ &= \frac{2 - 2}{2} = 0 \end{aligned}$$

- The zero bond order indicates that there is no bonding between the helium atoms .
- So, helium molecule does not exist**

4. HELIUM MOLECULE (He_2^+) ION

- It is formed by the combination of helium atom (**He**) having electronic configuration $1s^2$ and a helium ion (**He⁺**) having electronic configuration $1s^1$
- The molecule (**He₂⁺**) has three electrons.
- Two of the three electrons are placed in $\sigma 1s$ bonding MO whereas the third electron is placed in $\sigma^* 1s$ antibonding MO .
- The value of bond order shows that **He₂⁺** molecule ion is stable.
- The **He₂⁺** molecule ion has been identified in gaseous phase.



- The molecular orbital electronic configuration of **He₂⁺** molecule is :



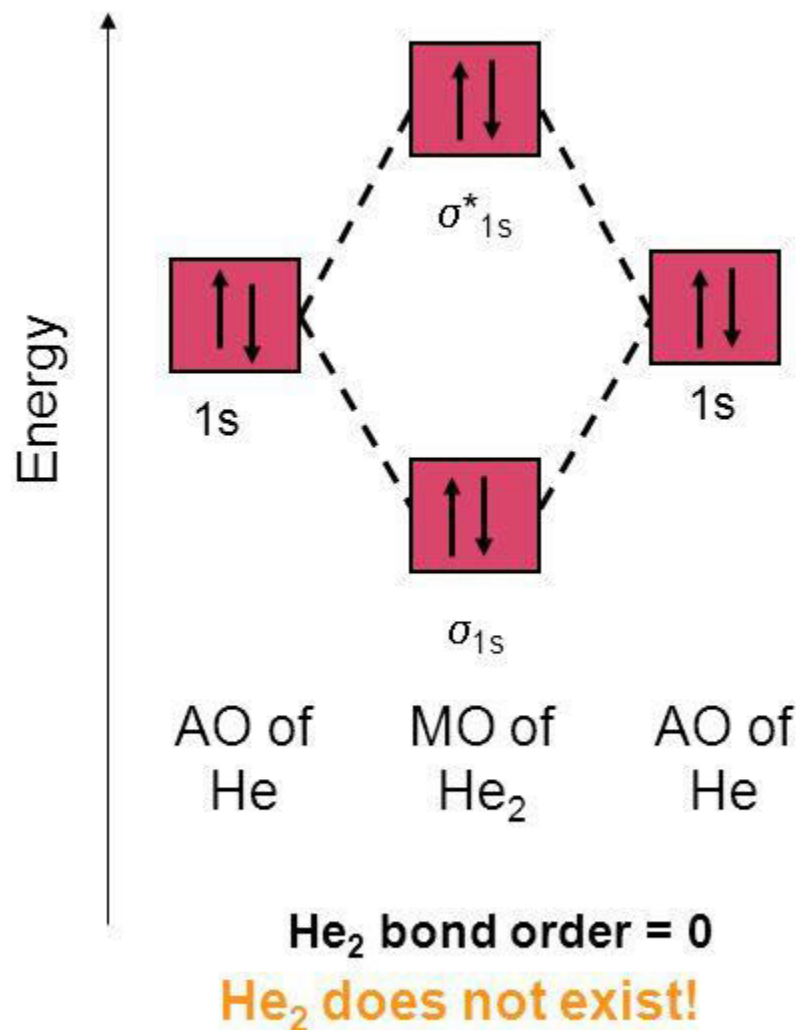
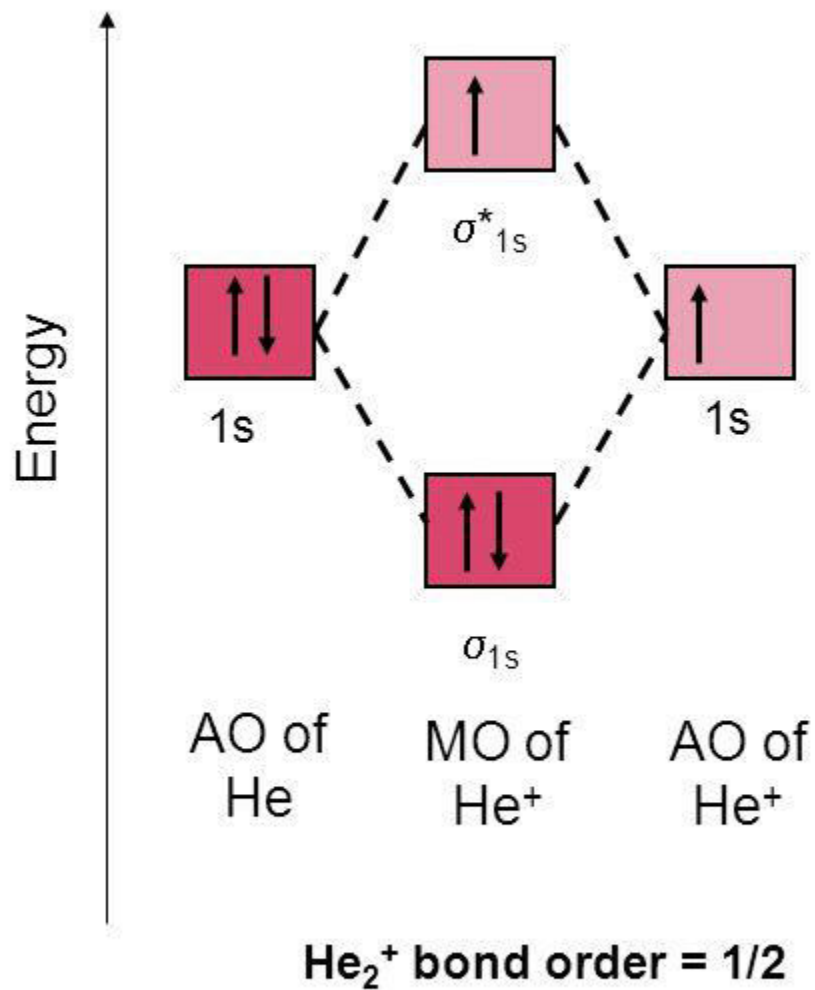
- The bond order is

$$\begin{aligned} \text{Bond order} &= \frac{N_b - N_a}{2} \\ &= \frac{2 - 1}{2} = \frac{1}{2} \end{aligned}$$

- Stable molecule ion
- B. D. Energy = 242 kJ/mol
- Paramagnetic in nature

Figure 11.16

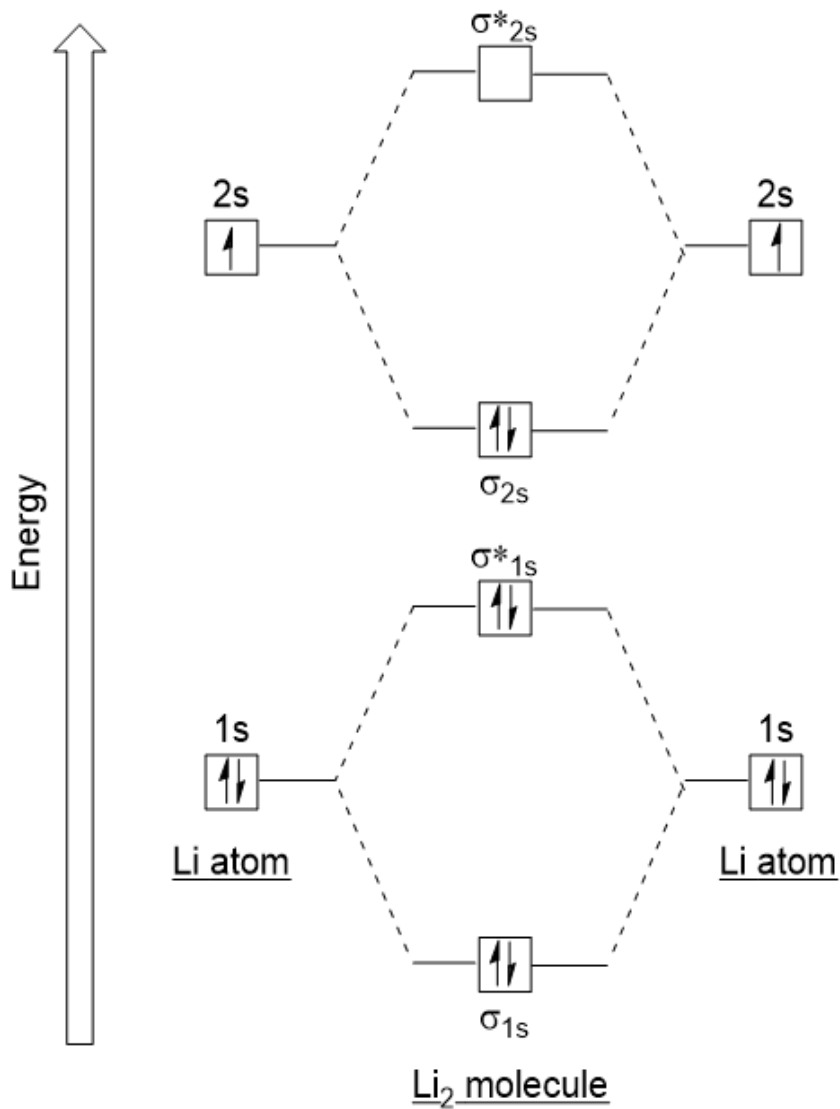
MO diagram for He_2^+ and He_2



5. LITHIUM MOLECULE (Li_2)

- It is formed by combination of two lithium atoms.
- The electronic configuration of each lithium atom ($Z = 3$) is $1s^2 2s^1$.
- Both the lithium atoms contribute six electrons towards bond formation.
- Four of these electrons are placed in the $\sigma 1s$ and $\sigma^* 1s$ molecular orbitals.
- The bonding effect of $\sigma 1s$ is completely cancelled by the antibonding effect of $\sigma^* 1s$. So, these four electrons do not contribute towards bonding at all.

- The remaining two electrons go to σ_{2s} bonding molecular orbitals.



- The molecular orbital electronic configuration of Li_2 molecule is :



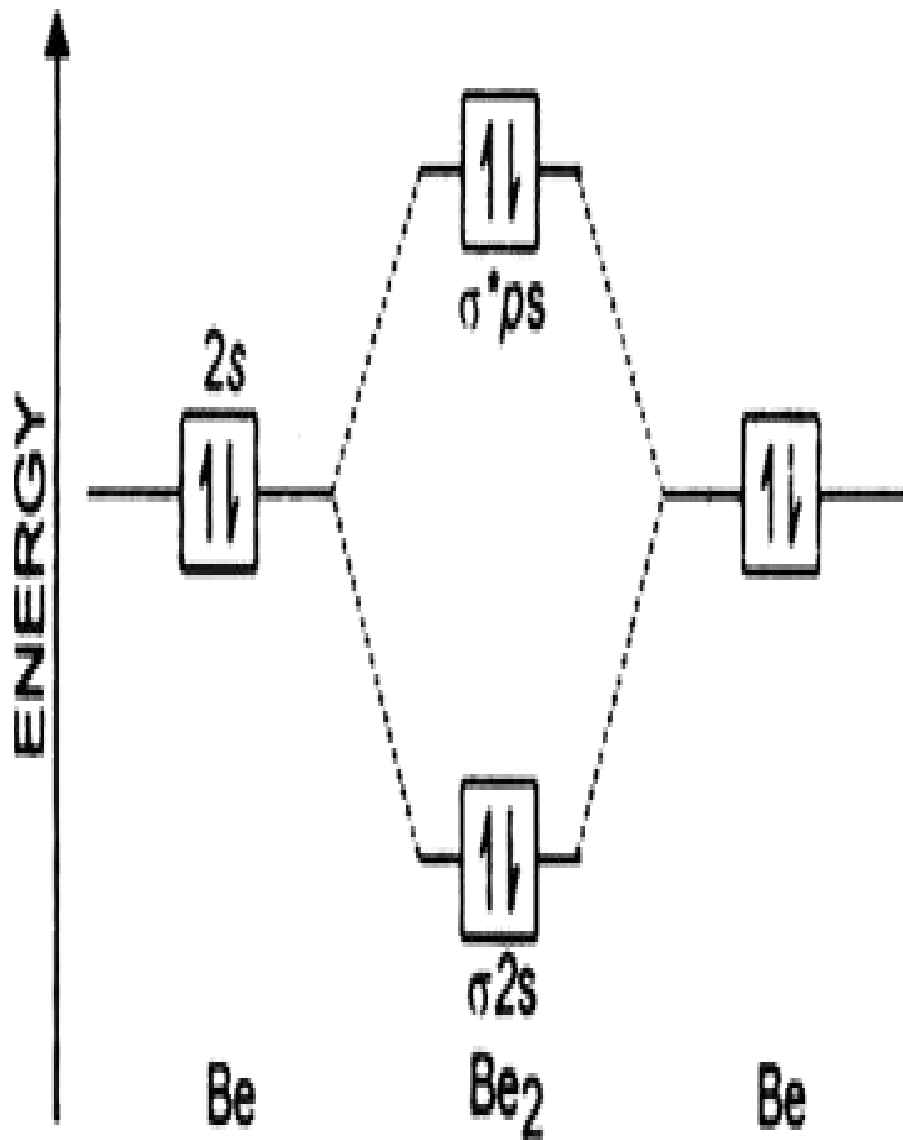
- The bond order is

$$\begin{aligned} \text{Bond order} &= \frac{N_b - N_a}{2} \\ &= \frac{2 - 0}{2} = 1 \end{aligned}$$

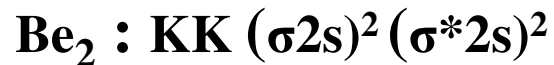
- Bond order value shows only one sigma bond.
- B. D. Energy = 105 kJ/mol (**Low**)
- Bond length = 2.67 Å
- Diamagnetic in nature

6. BERYLLIUM MOLECULE (Be_2)

- It is formed by combination of two beryllium atoms.
- The electronic configuration of each beryllium atom ($Z = 4$) is $1s^2 2s^2$.
- Both the beryllium atoms contribute eight electrons towards bond formation.
- Four of these electrons are placed in the σ_{1s} and σ^*_{1s} molecular orbitals and they do not contribute towards bonding as in case of lithium molecule.
- Out of the remaining four electrons, two electrons go to σ_{2s} BMO and the other two electrons go to σ^*_{2s} ABMOs.



- The molecular orbital electronic configuration of **Be₂** molecule is :



- The bond order is

$$\begin{aligned} \text{Bond order} &= \frac{N_b - N_a}{2} \\ &= \frac{2 - 0}{2} = 0 \end{aligned}$$

- Bond order value is zero, which indicates that beryllium molecule does not exist

7. BORON MOLECULE (B_2)

- The electronic configuration of each boron atom ($Z = 5$) is $1s^2 2s^2 2p^1$.
- Both the boron atoms contribute ten electrons towards bond formation.
- Four of these electrons are placed in the σ_{1s} and σ^*_{1s} molecular orbitals and they do not contribute towards bonding as in case of lithium molecule.
- The other six electrons are to be placed in other molecular orbitals. Two electrons go to σ_{2s} BMO and the other two electrons go to σ^*_{2s} ABMOs.

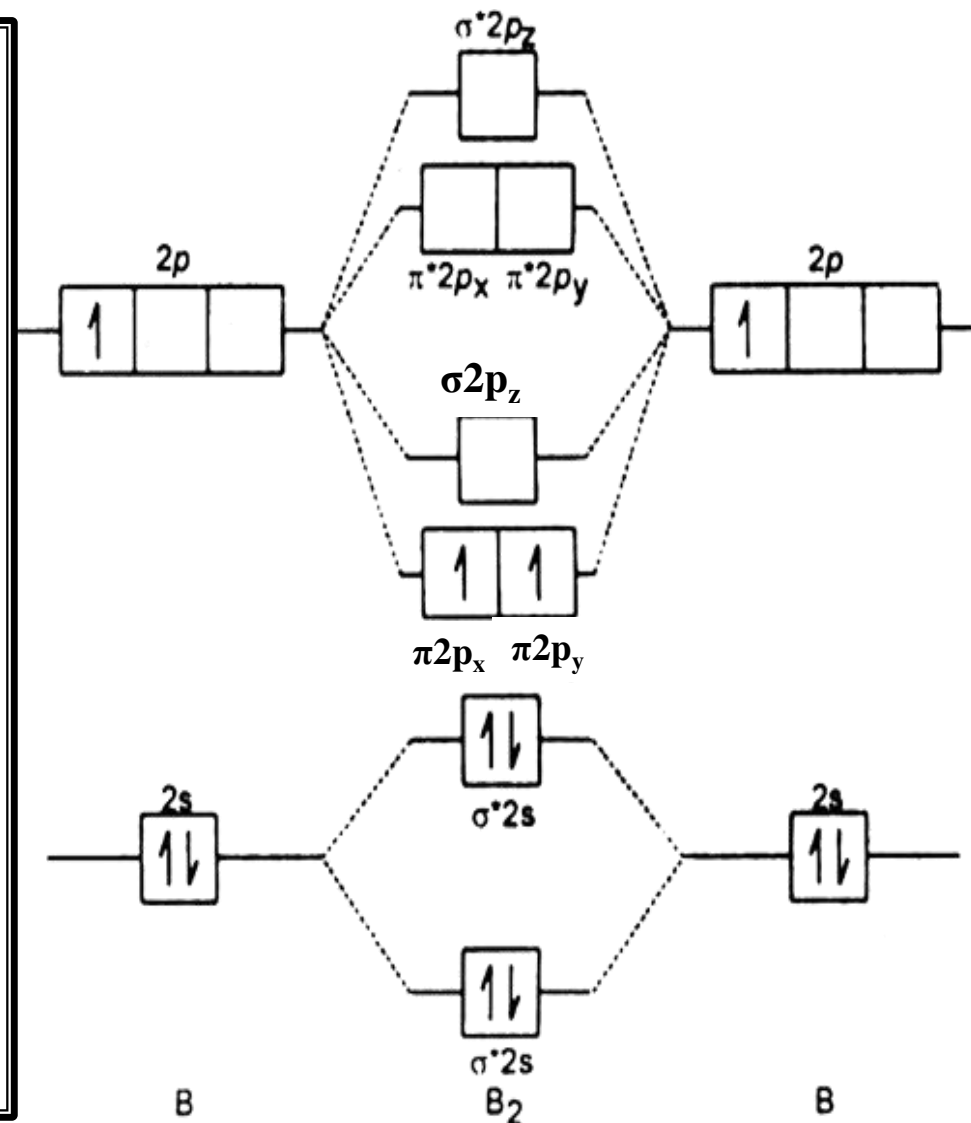
- The remaining two electrons are placed in $\pi 2p_x$ and $\pi 2p_y$ BMOs of equal energy

The molecular orbital electronic configuration of B_2 molecule is :
 $B_2 : KK (\sigma 2s)^2 (\sigma^* 2s)^2 (\pi 2p_x)^1 (\pi 2p_y)^1$

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

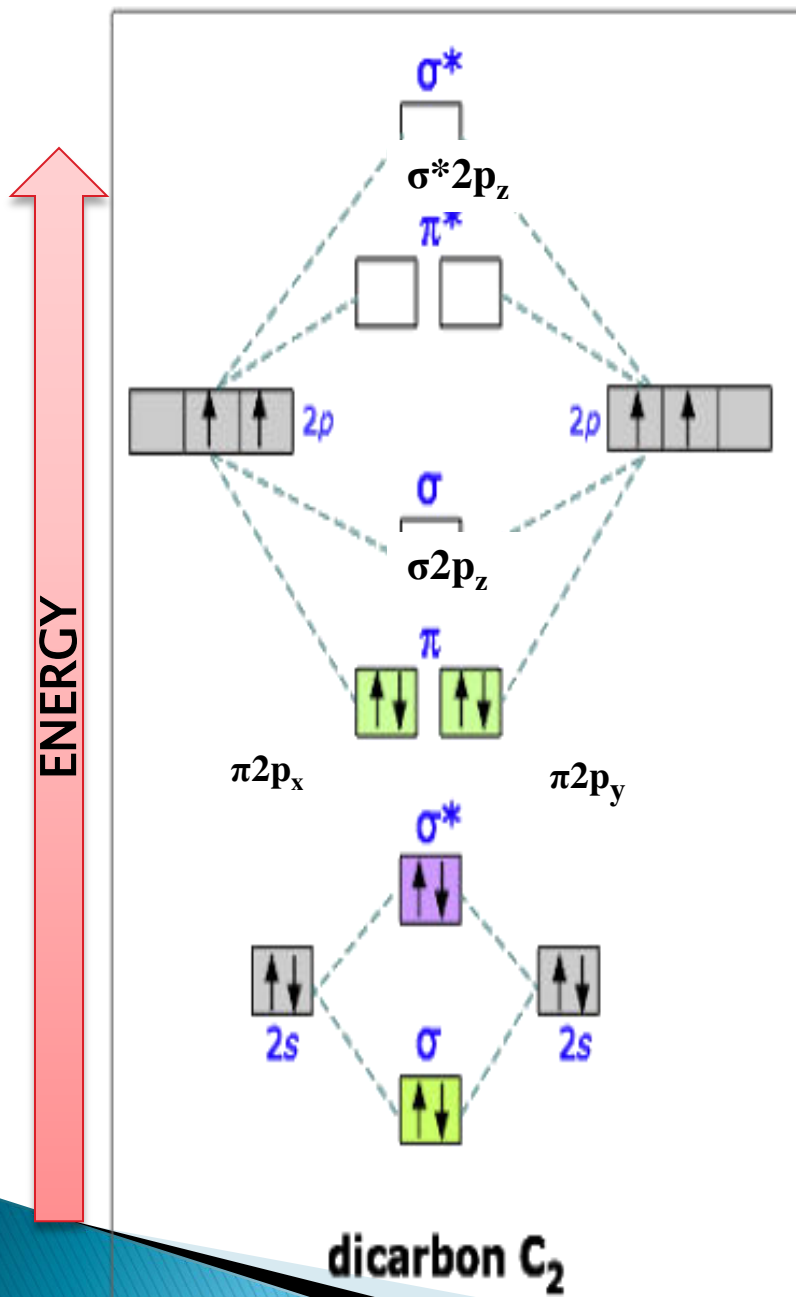
$$= \frac{4 - 2}{2} = 1$$

- The molecule has only one bond.
- The electrons which contribute to bonding are $(\pi 2p_x)^1 (\pi 2p_y)^1$. The molecule is formed by a weak π bond.
- B. D. Energy = 272kJ/mol**
- Bond length = 1.59 Å**
- Paramagnetic in nature**



8. CARBON MOLECULE (C_2)

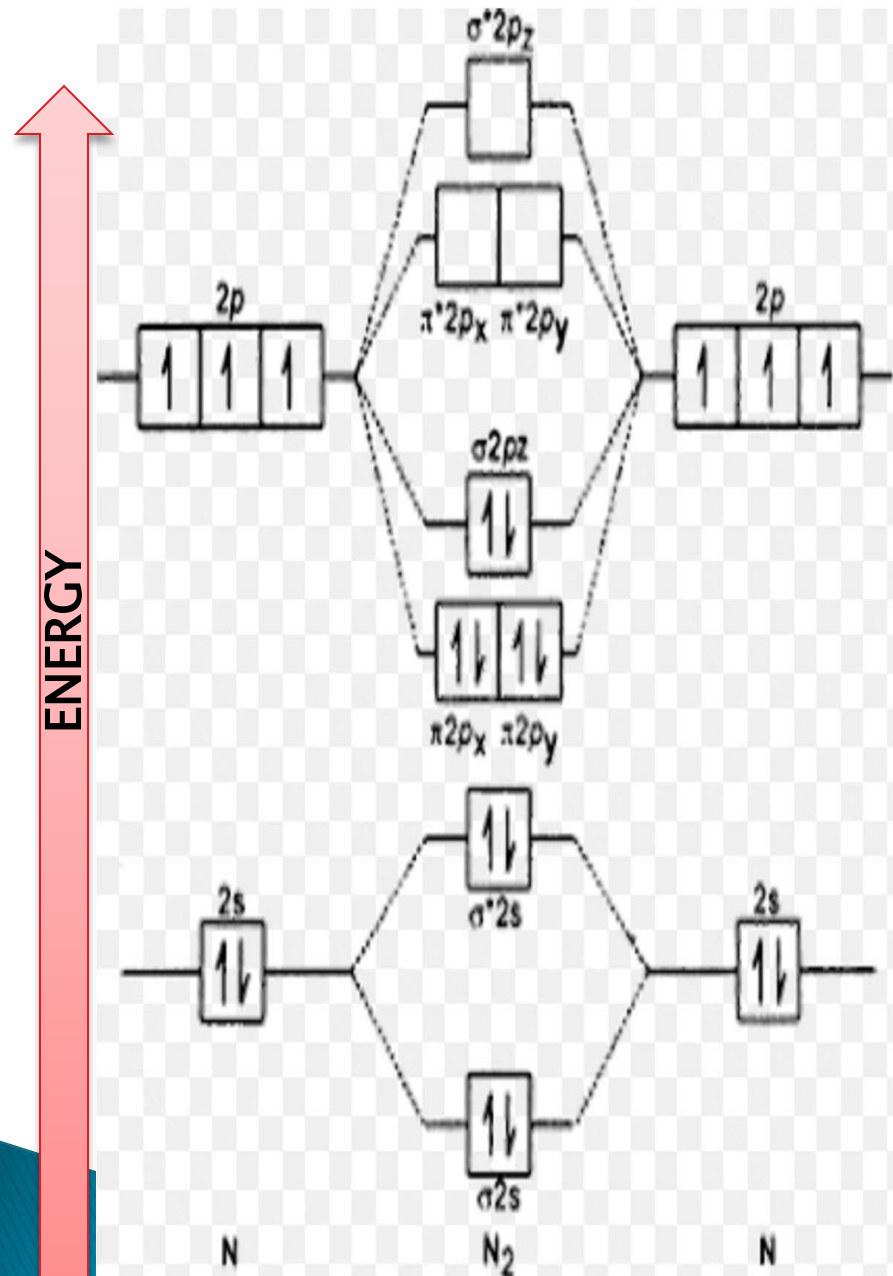
- The electronic configuration of each carbon atom ($Z = 6$) is $1s^2 2s^2 2p^2$.
- Ignoring the inner $1s$ electrons as they do not contribute towards bonding as in earlier cases.
- Both the carbon atoms contribute **eight electrons** (valence shell electrons) to be placed in outer molecular orbitals of C_2 .
- Four of these electrons are placed in the $\sigma 2s$ and $\sigma^* 2s$ MOs.
- The remaining four electrons are placed in $\pi 2p_x$ and $\pi 2p_y$ **BMOs** of equal energy. These orbitals are completely filled



- The molecular orbital electronic configuration of C_2 molecule is :
 $C_2 : KK (\sigma 2s)^2 (\sigma^* 2s)^2 (\pi 2p_x)^2 (\pi 2p_y)^2$
- Bond order = $\frac{N_b - N_a}{2}$
 $= \frac{6 - 2}{2} = 2$
- The C_2 molecule has two bonds.
- The electrons which contribute to bonding are $(\pi 2p_x)^2 (\pi 2p_y)^2$.
- **B. D. Energy = 602kJ/mol**
- **Bond length = 1.31 Å**
- **Diamagnetic in nature**

9. NITROGEN MOLECULE (N_2)

- The electronic configuration of each nitrogen atom ($Z = 7$) is $1s^2 2s^2 2p^3$.
- The number of valence electrons per nitrogen atom is **5**.
- Both the nitrogen atoms contribute **ten electrons** (valence shell electrons) to be placed in outer molecular orbitals of N_2 .
- Four of these electrons are placed in the **$\sigma 2s$ and $\sigma^* 2s$** MOs.
- Out of the six, four electrons are placed in **$\pi 2p_x$ and $\pi 2p_y$** BMOs of equal energy. The **remaining two electrons** are placed in **higher energy $\sigma 2p_z$** bonding molecular orbital.



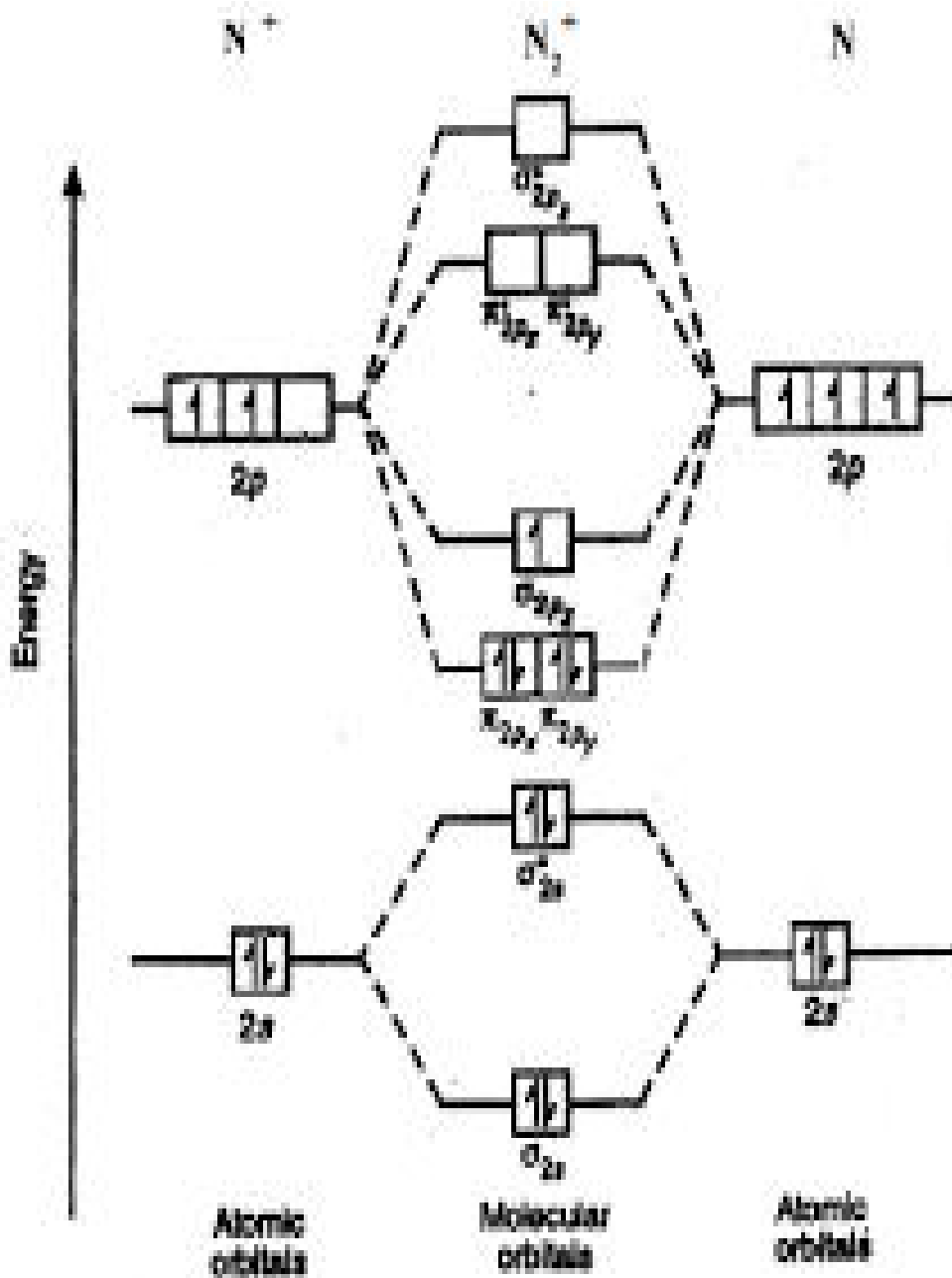
- The molecular orbital electronic configuration of N_2 molecule is :
 $N_2 : KK (\sigma_{2s})^2 (\sigma^*_{2s})^2 (\pi_{2p_x})^2 (\pi_{2p_y})^2 (\sigma_{2p_z})^2$

- Bond order = $\frac{N_b - N_a}{2}$
 $= \frac{8 - 2}{2} = 3$

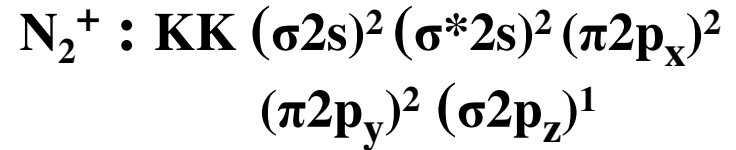
- The N_2 molecule has a **triple bond**, one σ and two π bonds.
- The nitrogen molecule is highly stable due to triple bond.
- B. D. Energy = 941kJ/mol**
- Bond length = 1.10 Å**
- Diamagnetic in nature**

9a. NITROGEN MOLECULE (N_2^+) ION

- In cases, one of the nitrogen is taken as a atom whereas the other nitrogen is taken as an ion.
- Electronic configuration of **N atom** ($Z = 7$) is $1s^2 2s^2 2p^3$.
- Electronic configuration of **N^+ ion** ($Z = 7$) is $1s^2 2s^2 2p^2$
- Both the nitrogen atom and ion contribute **nine electrons** (valence electrons) to be placed in molecular orbitals of N_2^+ .
- Four of these electrons are placed in the **$\sigma 2s$ and $\sigma^* 2s$** MOs.
- Out of the five, four electrons are placed in **$\pi 2p_x$ and $\pi 2p_y$ BMOs** of equal energy. The **remaining one electron** is placed in **higher energy $\sigma 2p_z$ BMO**.



- The molecular orbital electronic configuration of N_2^+ molecule is :

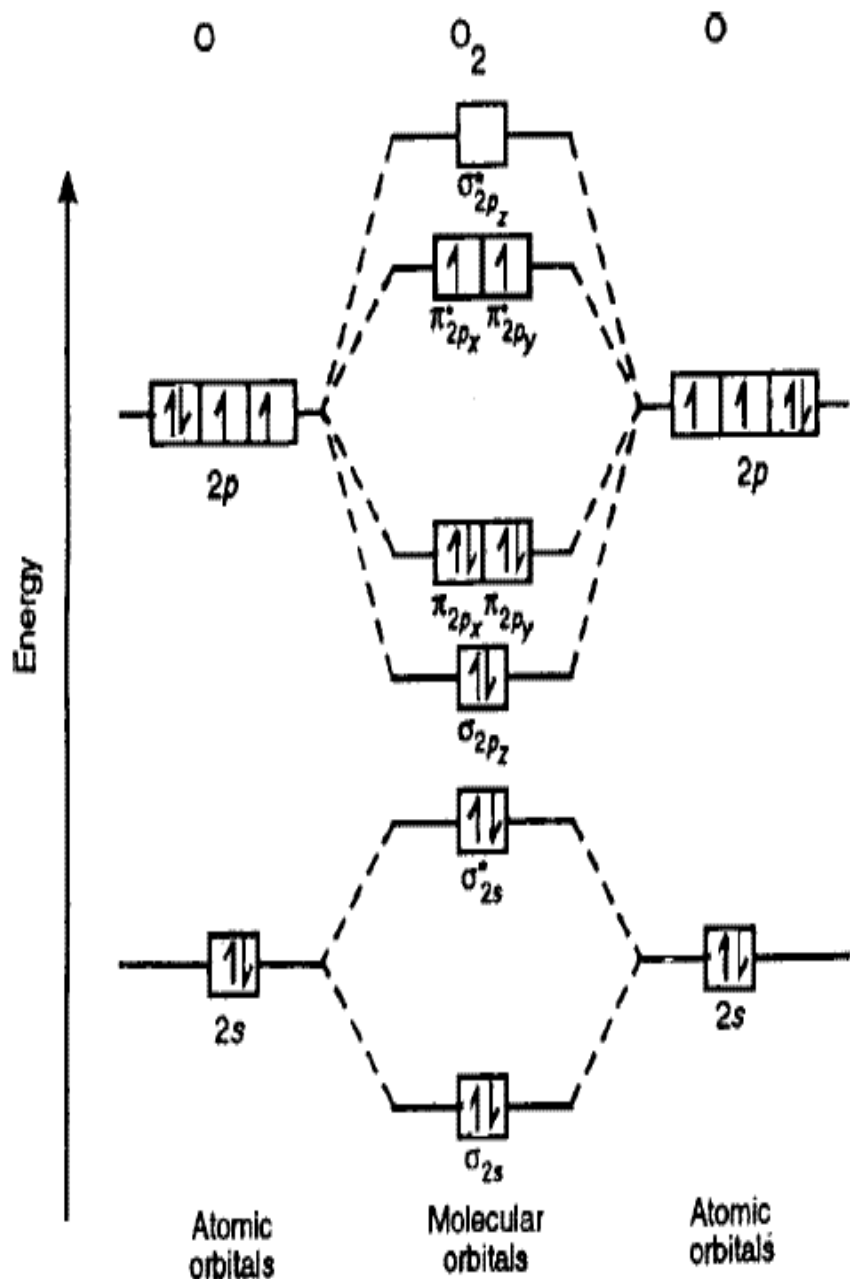


- Bond order = $\frac{N_b - N_a}{2}$
 $= \frac{7 - 2}{2} = 2.5$

- B. D. Energy** = $N_2^+ < N_2$.
- Bond length** = $N_2^+ > N_2$
- Paramagnetic in nature**

10. OXYGEN MOLECULE (O_2)

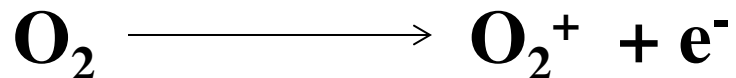
- The electronic configuration of each oxygen atom ($Z = 8$) is $1s^2 2s^2 2p^4$.
- The number of valence electrons per oxygen atom is **6**.
- Both the oxygen atoms contribute **twelve electrons** (valence electrons) to be placed in outer molecular orbitals of O_2 .
- **Four** of these electrons are placed in the σ_{2s} and σ^*_{2s} MOs.
- Out of the eight, **six electrons** are placed in σ_{2p_z} , π_{2p_x} and π_{2p_y} bonding molecular orbital.
- As all the BMOs are filled, the **remaining two electrons** are placed in $\pi^*_{2p_x}$ and $\pi^*_{2p_y}$ ABMOs.



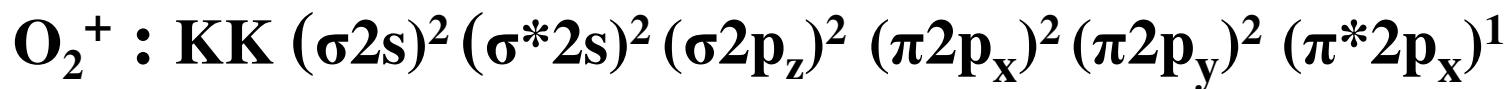
- The molecular orbital electronic configuration of O_2 molecule is :
 $O_2 : KK (\sigma 2s)^2 (\sigma^* 2s)^2 (\sigma 2p_z)^2 (\pi 2p_x)^2 (\pi 2p_y)^2 (\pi^* 2p_x)^1 (\pi^* 2p_y)^1$
- Bond order = $\frac{N_b - N_a}{2}$
 $= \frac{8 - 4}{2} = 2$
- The O_2 molecule has a **double bond**, one σ and one π bond.
- The last two electrons in $\pi^* 2p_x$ and $\pi^* 2p_y$ will remain unpaired (Hund's rule)
- **B. D. Energy = 493 kJ/mol**
- **Bond length = 1.21 Å**
- **Paramagnetic in nature**

COMPARISON OF O_2 , O_2^+ , O_2^- SPECIES

- O_2^+ ion is formed by removing one electron from O_2 molecule.

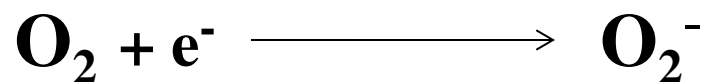


- The electron will be lost from antibonding π^*2p_y MO.
- The molecular orbital electronic configuration of O_2 molecule is :



- Bond order = $\frac{N_b - N_a}{2} = \frac{8 - 3}{2} = 2.5$
- Bond strength of $O_2^+ > O_2$ and bond length of $O_2^+ < O_2$

- O_2^- ion is formed by adding one electron to the O_2 molecule.

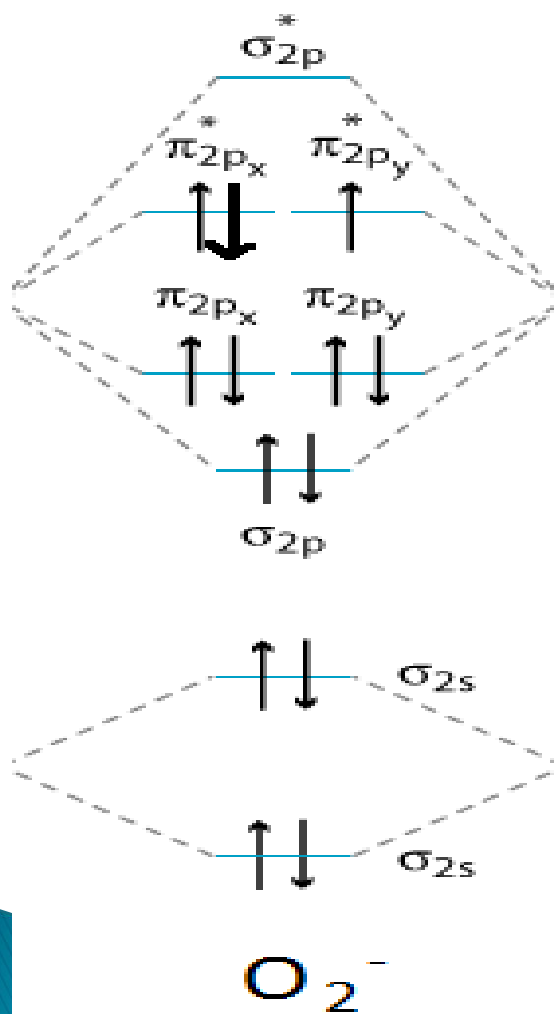


- The electron will be added to either π^*2p_x or π^*2p_y antibonding MO.
- The molecular orbital electronic configuration of O_2 molecule is $\text{O}_2^- : \text{KK} (\sigma 2s)^2 (\sigma^* 2s)^2 (\sigma 2p_z)^2 (\pi 2p_x)^2 (\pi 2p_y)^2 (\pi^* 2p_x)^2 (\pi^* 2p_x)^1$
- Bond order = $\frac{N_b - N_a}{2} = \frac{8 - 5}{2} = 1.5$
- Bond strength of $\text{O}_2^- < \text{O}_2$ and bond length of $\text{O}_2^- > \text{O}_2$

B.O = 1.5

B.S = $O_2^- < O_2$

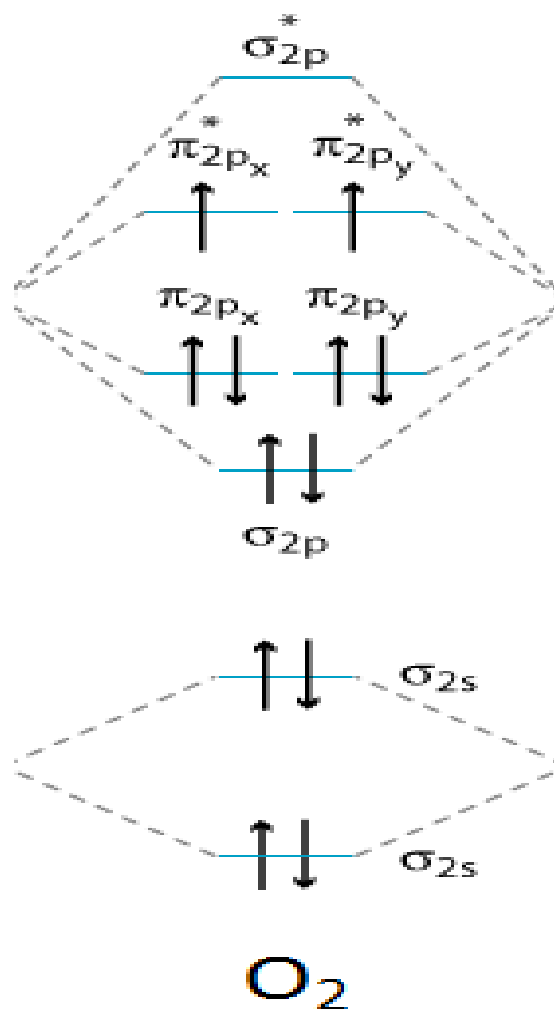
B.D.E = ----



B.O = 2

B.S = $O_2^+ > O_2 > O_2^-$

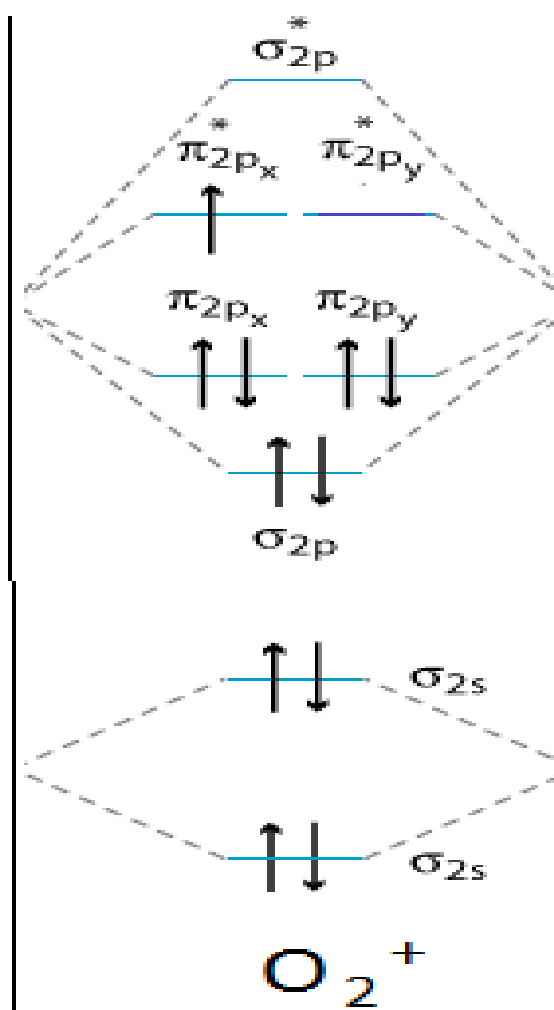
B.D.E = 493 kJ/mol



B.O = 2.5

B.S = $O_2^+ > O_2$

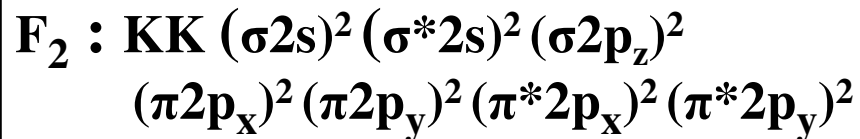
B.D.E = 625 kJ/mol



11. FLUORINE MOLECULE (F_2)

- The electronic configuration of each fluorine atom ($Z = 9$) is $1s^2 2s^2 2p^5$.
- The number of valence electrons per fluorine atom is 7.
- Both the fluorine atoms contribute **fourteen electrons** (valence electrons) to be placed in molecular orbitals of F_2 .
- **Four** of these electrons are placed in the $\sigma 2s$ and $\sigma^* 2s$ MOs.
- Out of the ten, **six electrons** are placed in $\sigma 2p_z$, $\pi 2p_x$ and $\pi 2p_y$ bonding molecular orbital.
- As all the BMOs are filled, the **remaining four electrons** are placed in $\pi^* 2p_x$ and $\pi^* 2p_y$ ABMOs.

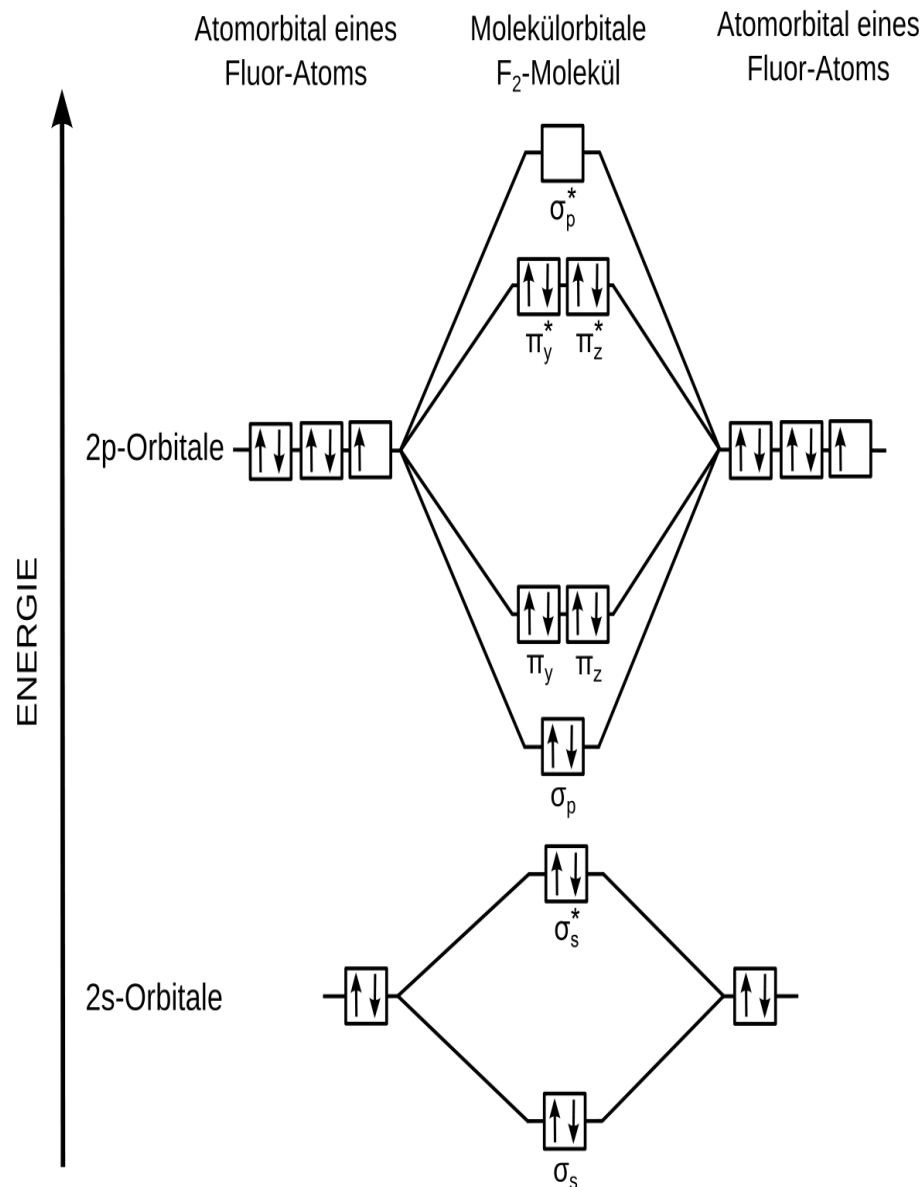
- The molecular orbital electronic configuration of F_2 molecule is :



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

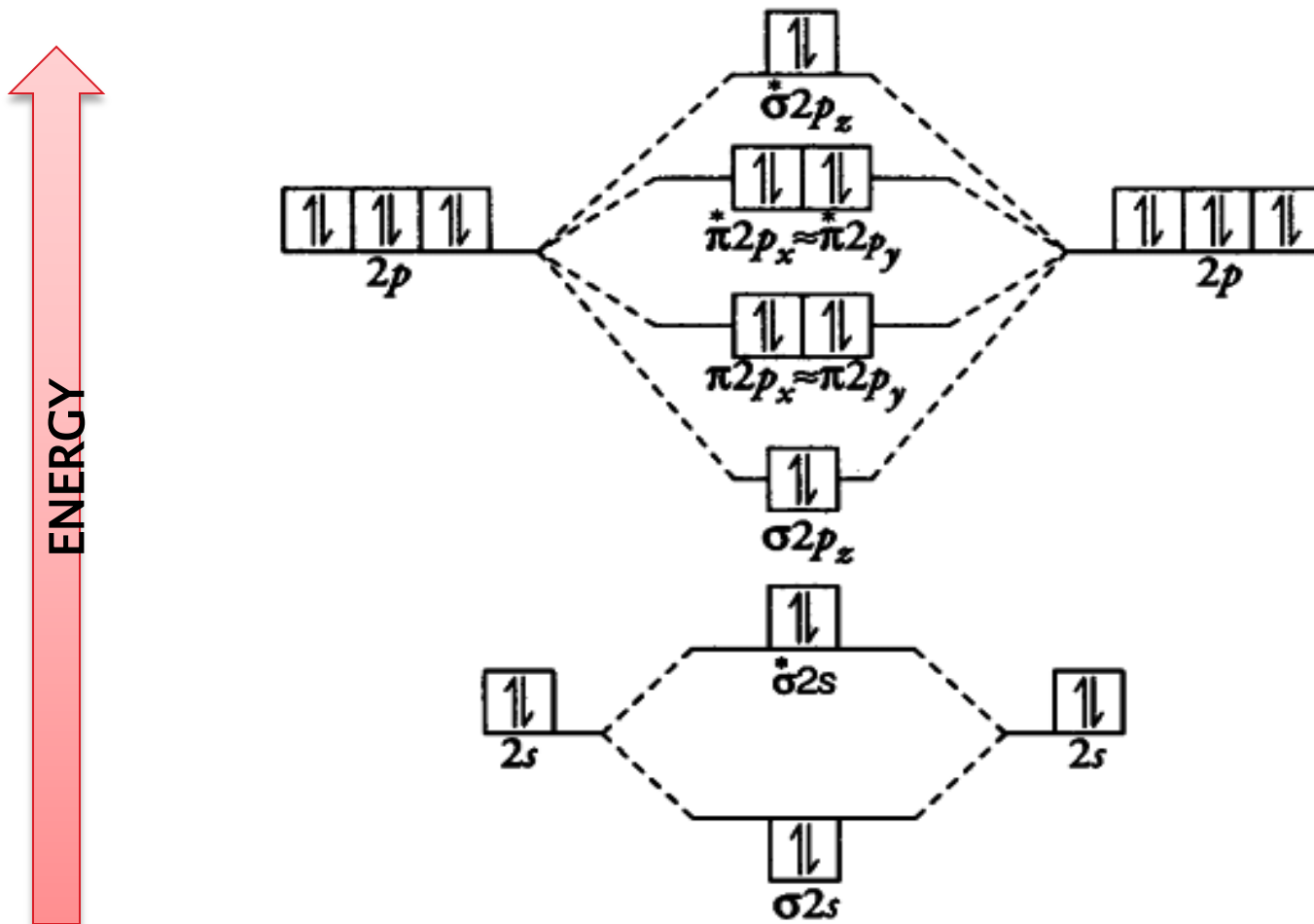
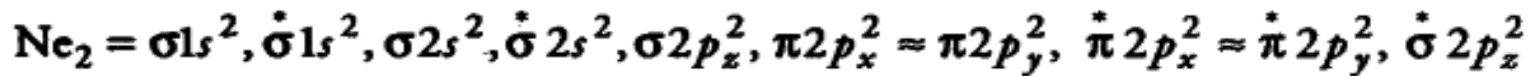
$$= \frac{8 - 6}{2} = 1$$

- The F_2 molecule has a **single σ bond**.
- The presence of **6 electrons in ABMOs** make fluorine **weaker** than oxygen
- B. D. Energy = 140 kJ/mol**
- Bond length = 1.42 Å**
- Diamagnetic in nature**



12. NEON MOLECULE (Ne_2)

- The electronic configuration of each neon atom ($Z = 10$) is $1s^2 2s^2 2p^6$.
- The number of valence electrons per neon atom is **8**.
- Both the neon atoms contribute **sixteen electrons** (valence electrons) to be placed in molecular orbitals of Ne_2 .
- **Four** of these electrons are placed in the $\sigma 2s$ and $\sigma^* 2s$ MOs.
- Out of the twelve, **six electrons** are placed in $\sigma 2p_z$, $\pi 2p_x$ and $\pi 2p_y$ bonding molecular orbital.
- As all the BMOs are filled, the **remaining six electrons** are placed in $\pi^* 2p_x$, $\pi^* 2p_y$, $\sigma^* 2p_z$ ABMOs.



Bond order = $\frac{1}{2}(8 - 8) = 0$. So, Ne_2 molecule does not exist

M.O. ENERGY LEVEL DIAGRAM FOR HETERONUCLEAR DIATOMIC MOLECULES

- The MOT can be extended to heteronuclear diatomic molecules.
- Consider a heteronuclear diatomic molecule **AB** in which **B** is **more electronegative** than A.
- The MO obtained by the combination of atom A and B can be written as:

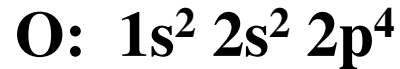
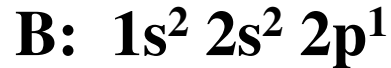
$$\psi = C_A \psi_A + C_B \psi_B$$

where C_A and C_B are the mixing coefficients and ψ_A and ψ_B are the wave functions associated with atom A and B

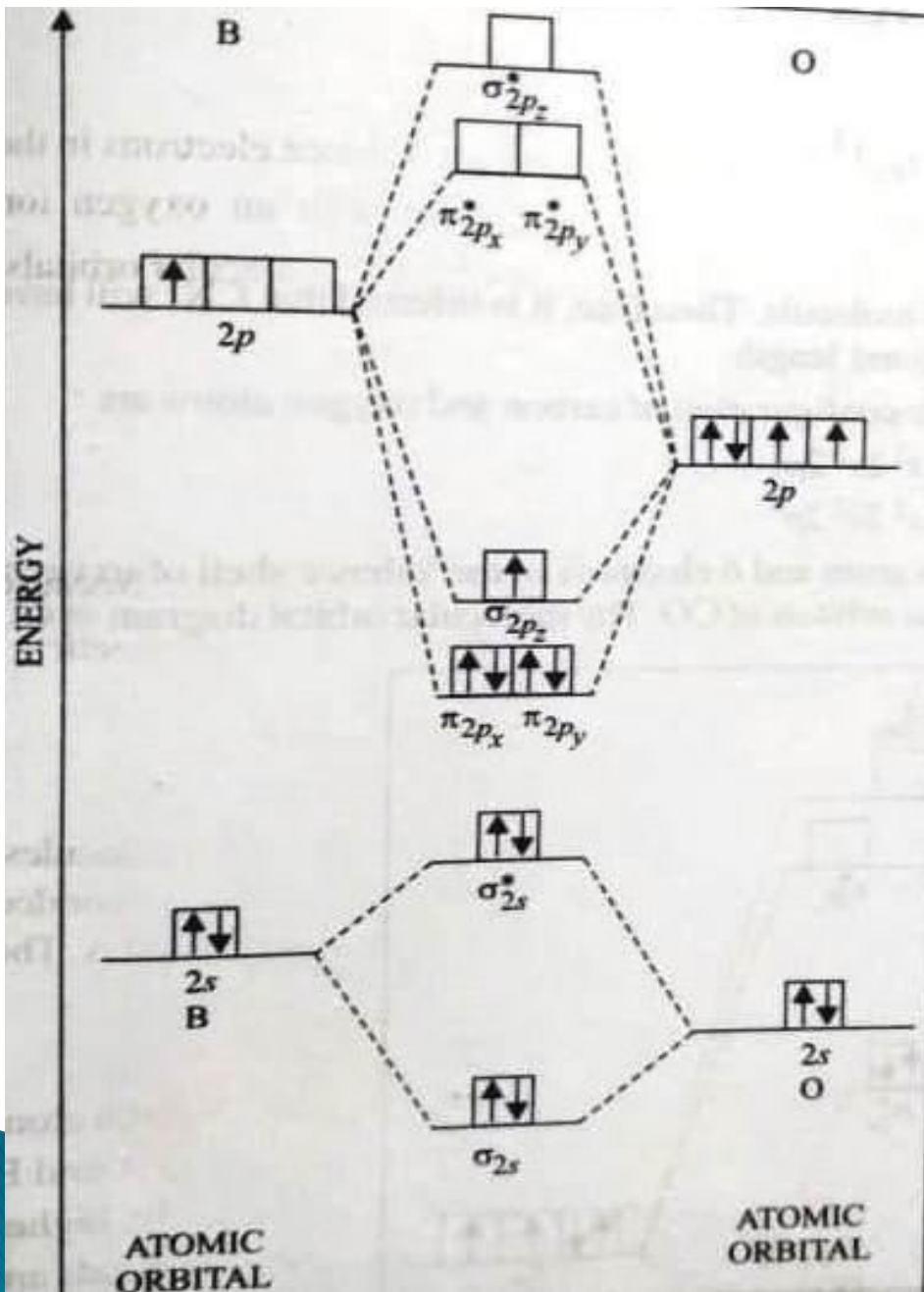
- The values of coefficient C_A and C_B in the above equation are different as A and B are two different atoms.
- The atomic orbitals of atoms A and B are placed at different levels.
- The atom with higher electronegativity will have lower energy than the other atom.
- As B is more electronegative than A, the atomic orbitals of B are **placed lower in energy** than the corresponding orbitals of A.
- The BMO are **nearer to the more electronegative atom** whereas the ABMO are **closer to the less electronegative atom**.

1. BORON OXIDE (BO) MOLECULE

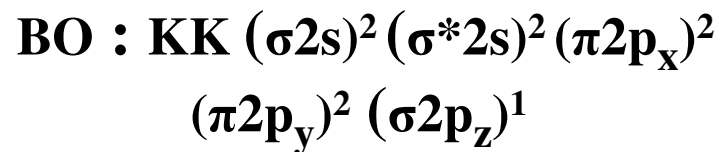
- The electronic configuration of boron and oxygen is



- There are a total of **9 valence electrons** (3 in the valence shell of boron and 6 in the valence shell of oxygen) that are to be placed in the MO's of Boron oxide.
- As Oxygen is more electronegative than Boron, the 2s and 2p orbitals of oxygen are **lower in energy** than the corresponding orbitals of boron.
- The BMO will be closer to oxygen and the ABMO will be near boron.



- The molecular orbital electronic configuration of **BO** molecule is :



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

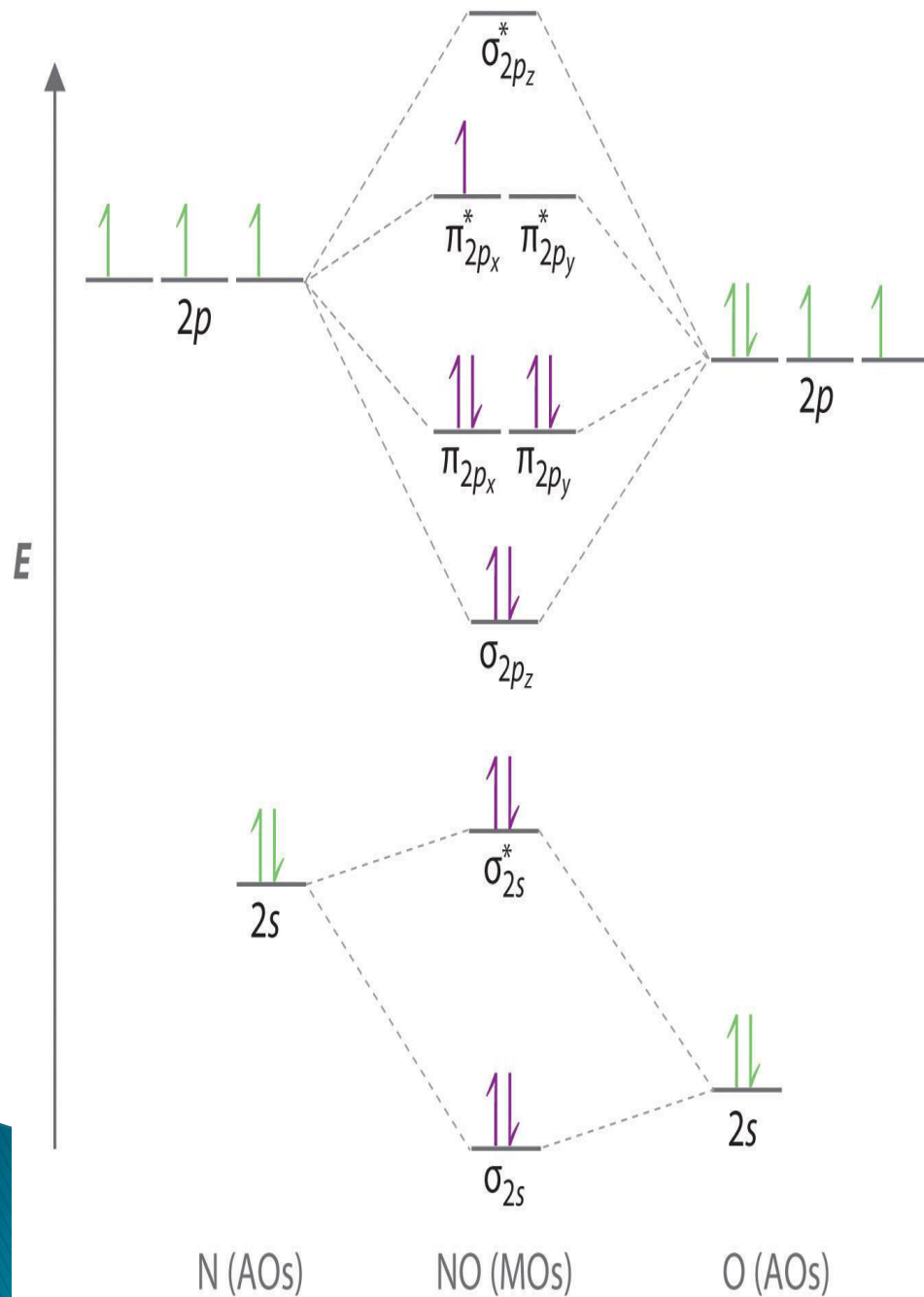
$$= \frac{7 - 2}{2} = 2.5$$
- B. D. Energy = 773.0 kJ/mol**
- Bond length = 1.20 Å**
- Paramagnetic in nature**

2. NITRIC OXIDE (NO) MOLECULE

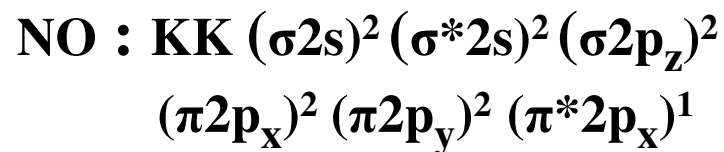
- The electronic configuration of nitrogen and oxygen is



- There are a total of 11 electrons (5 in the valence shell of nitrogen and 6 in the valence shell of oxygen) that are to be placed in the MO's of Nitrogen oxide.
- As Oxygen is more electronegative than nitrogen the 2s and 2p atomic orbitals of oxygen are lower in energy than the corresponding orbitals of nitrogen.
- The BMO will be closer to oxygen and the ABMO will be near nitrogen atom.



- The molecular orbital electronic configuration of **NO** molecule is :

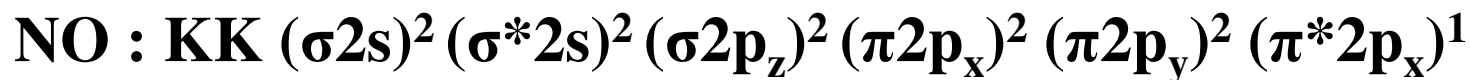


- Bond order = $\frac{N_b - N_a}{2}$
$$= \frac{8 - 3}{2} = 2.5$$

- B. D. Energy = 667.8 kJ/mol**
- Paramagnetic in nature**

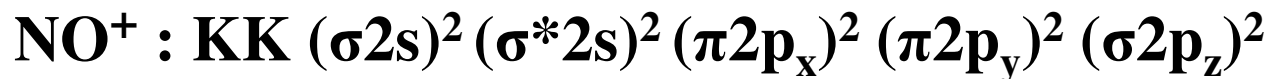
COMPARISON OF NO, NO⁺ and NO⁻

- The molecular orbital electronic configuration of **NO** molecule is :



$$\text{Bond order} = \frac{N_b - N_a}{2} = \frac{8 - 3}{2} = 2.5$$

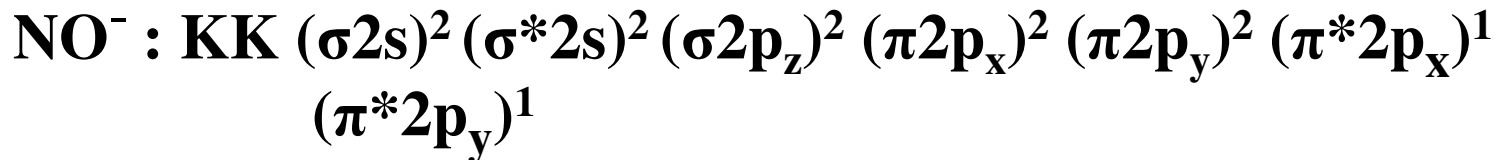
- In case of **NO⁺** one electron is removed from ABMO $\pi^* 2p_x$



$$\text{Bond order} = \frac{N_b - N_a}{2} = \frac{8 - 2}{2} = 3$$

So, the bond order of **NO⁺ > NO**. Bond dissociation energy is **more than** NO whereas bond length **will be less** than NO.

- In case of NO^- one electron is added to ABMO π^*2p_y



$$\text{Bond order} = \frac{N_b - N_a}{2} = \frac{8 - 4}{2} = 2$$

So, the bond order of $\text{NO}^- < \text{NO}$. Bond dissociation energy is **less than** NO whereas bond length **will be more** than NO.

- Thus the species NO , NO^+ and NO^- can be arranged in decreasing order of bond order as:



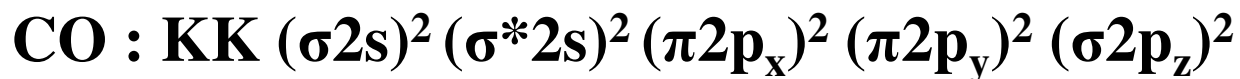
3. CARBON MONOXIDE (CO) MOLECULE

- The electronic configuration of carbon and oxygen atoms are



- There are a total of 10 electrons (4 in the valence shell of carbon and 6 in the valence shell of oxygen) that are to be placed in the MO's of Carbon monoxide molecule.
- As Oxygen is more electronegative than carbon the 2s and 2p atomic orbitals of oxygen are lower in energy than the corresponding orbitals of carbon.
- The BMO will be closer to oxygen and the ABMO will be near carbon atom.

- The molecular orbital electronic configuration of CO molecule is :

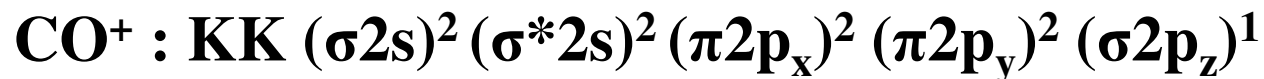


- Bond order = $\frac{N_b - N_a}{2} = \frac{8 - 2}{2} = 3$
- Triple bond
- B. D. Energy = 1067 kJ/mol
- Bond length = 1.128 Å
- Diamagnetic in nature
- Molecular orbital diagram for CO molecule is more complicated as can be seen when **CO** and **CO⁺** are compared.

COMPARISON OF CO and CO⁺

CO⁺ is formed by loss of one electron from CO molecule.

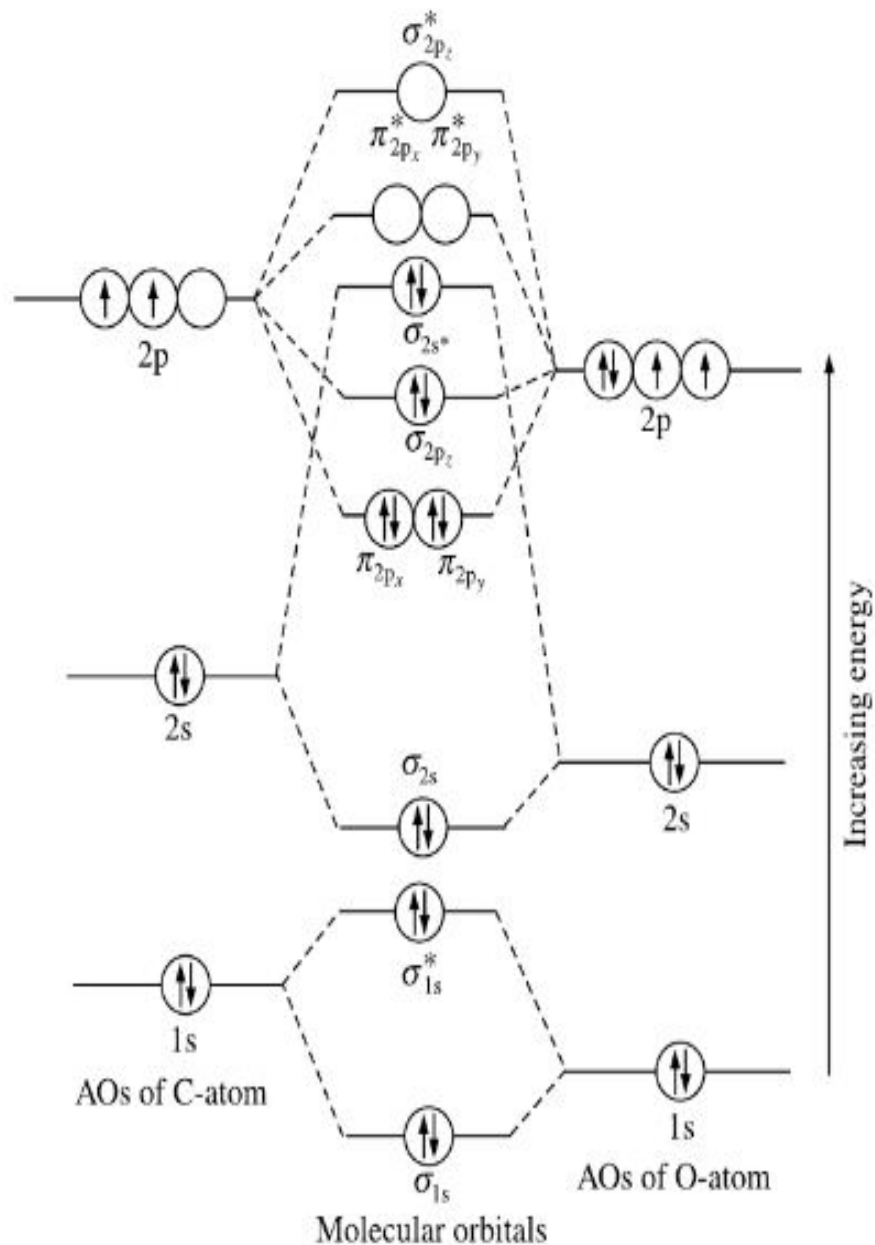
If the electronic configuration of CO molecule is correct, then the electronic configuration for CO⁺ is :



$$\text{Bond order} = \frac{N_b - N_a}{2} = \frac{7 - 2}{2} = 2.5$$

The bond order of CO⁺ should be reduced to 2.5 and the bond length should be more than CO molecule, but it was seen that the bond length of CO⁺ was 1.115Å which was less than that of CO molecule(1.128Å). **It means that the MO diagram of CO being similar to that of NO is incorrect.**

- It was seen that there is an **increase in bond order** when CO molecule changes to **CO⁺** ion.
- The decrease in bond length or increase in bond order of **CO⁺** **will only occur if the electron is removed** from an **ABMO** of CO molecule.
- This can be explained on the basis of energy levels of carbon and oxygen atoms.
- Oxygen being more electronegative than carbon, the AO's of oxygen are lower than those of carbon.
- This results in σ^*2s molecular orbital being higher in energy than $\sigma 2p_z$, $\pi 2p_x$, $\pi 2p_y$ molecular orbitals.



- As seen the σ^*2s MO is higher in energy than $\sigma2p_z$, $\pi2p_x$, $\pi2p_y$ MO's.
- For CO^+ , the electron is lost from σ^*2s MO and the bond order increases
- So, CO^+ has slightly stronger bond and smaller bond length than CO molecule.
- Electronic configuration for CO
 $\text{CO} : \text{KK} (\sigma2s)^2 (\pi2p_x)^2 (\pi2p_y)^2 (\sigma2p_z)^2 (\sigma^*2s)^2$
- Electronic configuration for CO^+
 $\text{CO}^+ : \text{KK} (\sigma2s)^2 (\pi2p_x)^2 (\pi2p_y)^2 (\sigma2p_z)^2 (\sigma^*2s)^1$

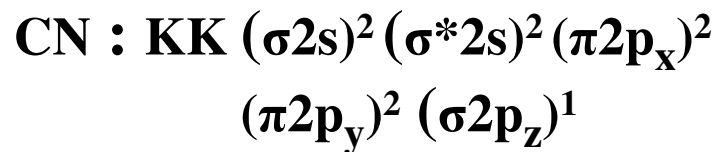
4. CYANIDE (CN) MOLECULE

- The electronic configuration of Carbon and Nitrogen atoms is



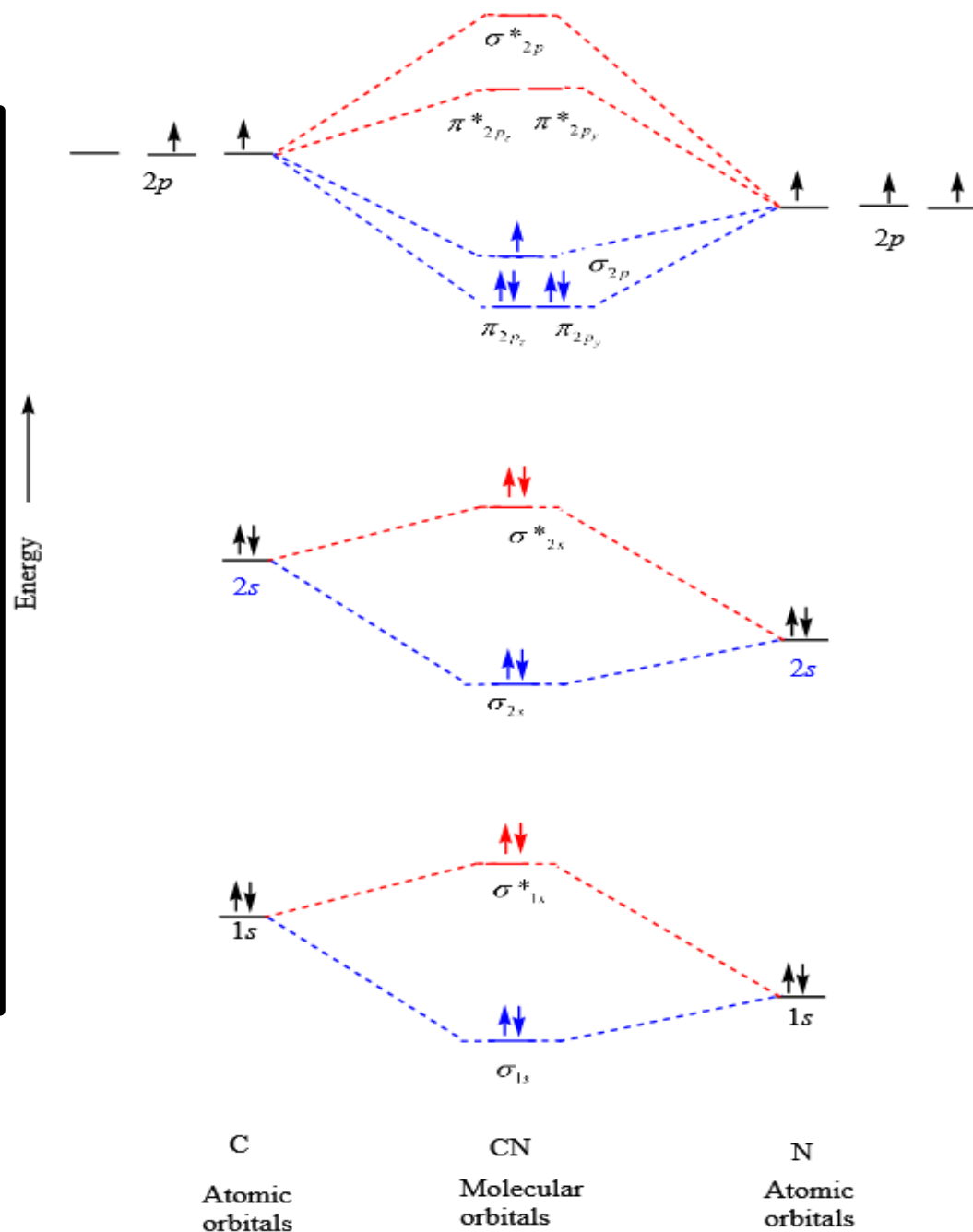
- There are a total of **9 electrons** (4 in the valence shell of carbon and 5 in the valence shell of nitrogen) that are to be placed in the MO's of Cyanide molecule.
- As Nitrogen is more electronegative than carbon, the 2s and 2p orbitals of nitrogen are lower in energy than the corresponding orbitals of carbon.
- The BMO will be closer to nitrogen and the ABMO will be near carbon atom.

- The molecular orbital electronic configuration of CN molecule is



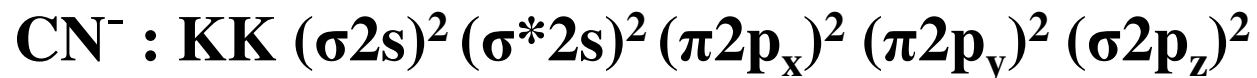
- Bond order = $\frac{N_b - N_a}{2}$
 $= \frac{7 - 2}{2} = 2.5$

- Paramagnetic in nature



COMPARISON OF CN and CN⁻

- In case of CN⁻ one electron is added to σ^*2p_z BMO of CN molecule



$$\text{Bond order} = \frac{N_b - N_a}{2} = \frac{8 - 2}{2} = 3$$

- So, the bond order of CN⁻ > CN. Bond dissociation energy of CN⁻ is **more than** CN whereas bond length **will be less** than CN.

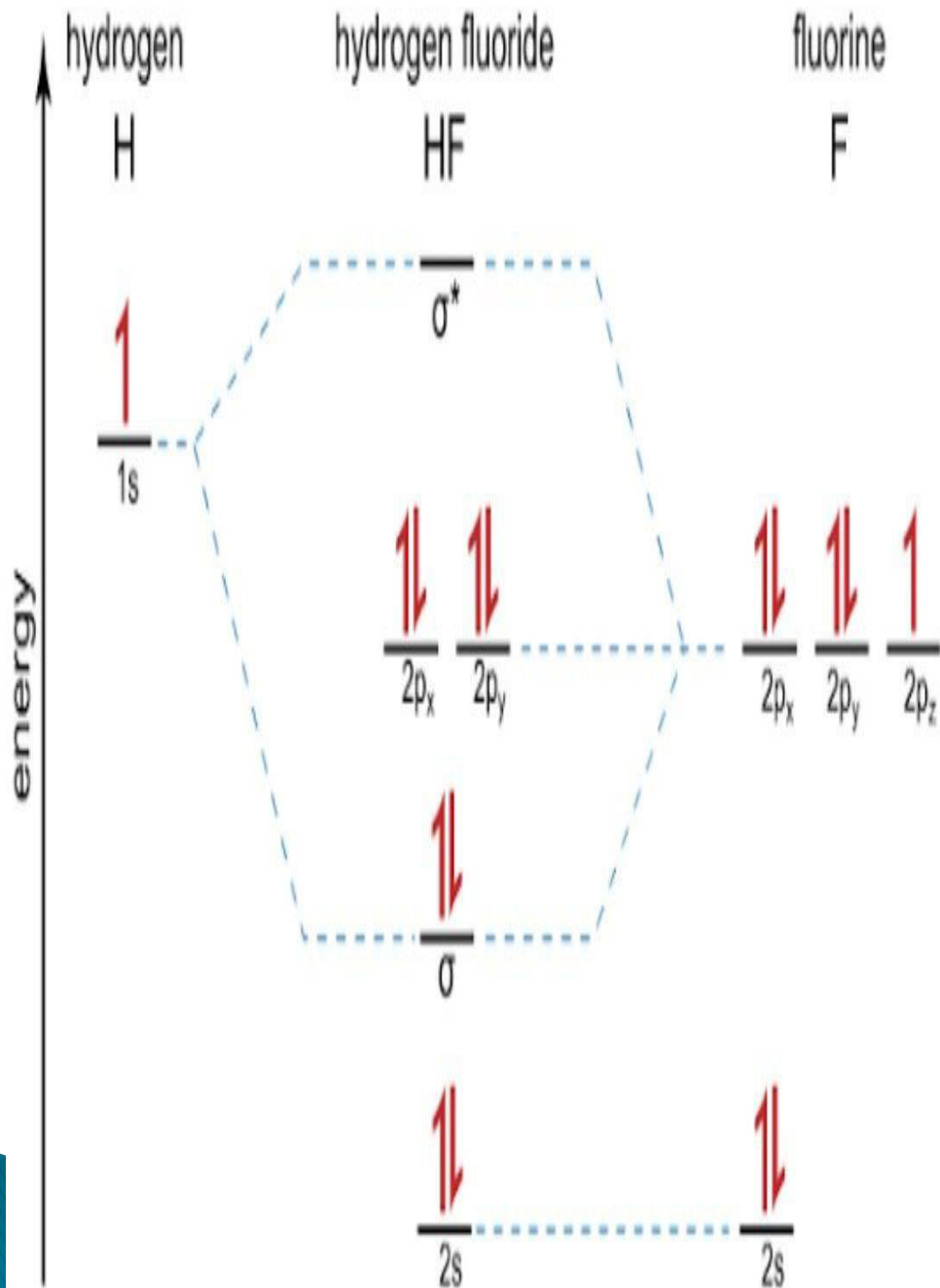
5. HYDROGEN FLUORIDE (HF) MOLECULE

- The electronic configuration of hydrogen and fluorine atom is



- Only the 2p orbital of fluorine will combine with 1s orbital of hydrogen.
- The 1s and 2s orbital of fluorine does not interact with 1s orbital of hydrogen as **they have low energies** and remain as atomic orbitals.
- Out of the three 2p orbitals of Nitrogen only **2p_z orbital** combines with 1s orbital of hydrogen because of **proper symmetry and energy**.

- The other two 2p orbitals ($2p_x$ and $2p_y$) **do not combine** with 1s orbital of hydrogen due to **improper symmetry and remain non bonding** molecular orbitals.
- The $2p_z$ orbital of fluorine combines with 1s orbital of hydrogen to form one bonding and one antibonding MO.
- These are represented as σ_{sp} and σ^*_{sp} respectively.
- Fluorine is more electronegative than hydrogen, so atomic orbitals of fluorine are lower in energy than that of hydrogen.
- Only two MO's (σ_{sp} and σ^*_{sp}) are formed.
- The remaining orbitals of fluorine atom remain **non - bonding**.



- The molecular orbital electronic configuration of **HF** molecule is



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

$$= \frac{2 - 0}{2} = 1$$

- Here **K** represents $1s^2$ of **Nitrogen**
- The electrons in the non bonding orbitals are not counted for calculating bond order.

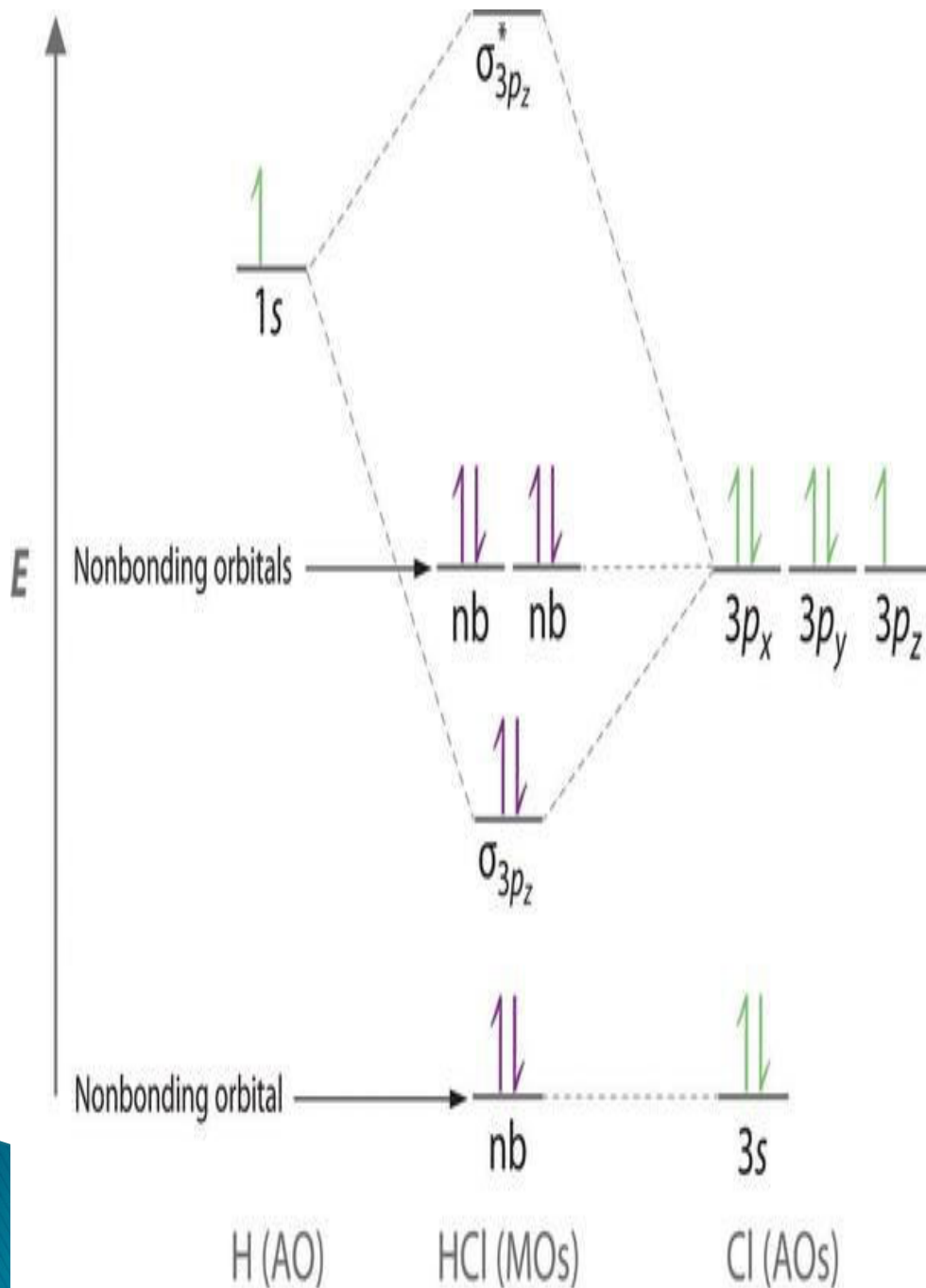
6. HYDROGEN CHLORIDE (HCl) MOLECULE

- The MO diagram for HCl molecule is similar to HF molecule.
- The electronic configuration of hydrogen and chlorine atom is



- Only the 3p orbital of chlorine will combine with 1s orbital of hydrogen.
- The 1s, 2s, 2p and 3s orbitals of chlorine do not interact with 1s orbital of hydrogen as **they have low energies** and remain as atomic orbitals.
- Out of the three 3p orbitals only **3p_z orbital** combines with 1s orbital of hydrogen because of **proper symmetry and energy**.

- The other two 3p orbitals ($3p_x$ and $3p_y$) of chlorine **do not combine** with 1s orbital of hydrogen due to **improper symmetry and remain non bonding** molecular orbitals.
- The $3p_z$ orbital of chlorine combines with 1s orbital of hydrogen to form one bonding and one antibonding MO.
- These are represented as σsp and $\sigma^* sp$ respectively.
- Chlorine is more electronegative than hydrogen, so atomic orbitals of chlorine are lower in energy than that of hydrogen.
- Only two MO's (σsp and $\sigma^* sp$) are formed.
- The remaining orbitals of chlorine atom remain non-bonding.



- The molecular orbital electronic configuration of **HCl** molecule is



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

$$= \frac{2 - 0}{2} = 1$$
- Here **K, L** represents inner shells of chlorine atom.
- The electrons in the non bonding orbitals are not counted for calculating bond order.

COMPARISON OF VALENCE BOND & MOLECULAR ORBITAL THEORY

SIMILARITIES

- Both theories are mere approximations.
- Both theories consider the overlapping of AO's for formation of a covalent bond.
- Both theories consider that interacting AO's should have nearly same energy and appropriate symmetry about the internuclear axis.
- Both theories predict the concentration of electron density between the nuclei.
- Both theories account for the directional nature of covalent bond.
- Both theories follow Pauli's exclusion principle, Hund's rule and Aufbau's rule for distribution of electrons.
- Both successfully explain the non existence of helium molecule.

DIFFERENCES

S.No	VALENCE BOND THEORY	MOLECULAR ORBITAL THEORY
1.	It starts with individual atoms and considers the interaction between them.	It starts with the nuclei of the constituting atoms.
2.	Electrons in molecules are localised as if they are present in individual atoms.	Electrons in molecules are delocalised over the whole molecule.
3.	Atoms retain their individual identity.	Atoms lose their individual identity.
4.	Involves the concept of resonance.	Does not involve the concept of resonance.
5.	It underestimates the ionic contribution in the total wave function.	It overestimates the ionic contribution in the total wave function.
6.	Fails to explain the paramagnetic nature of O_2 molecule.	Successfully explains the paramagnetic nature of O_2 molecule.

THANK

YOU