Molecular Orbital Diagram.

M.O. Diagram.

Molecular Orbital Configuration

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

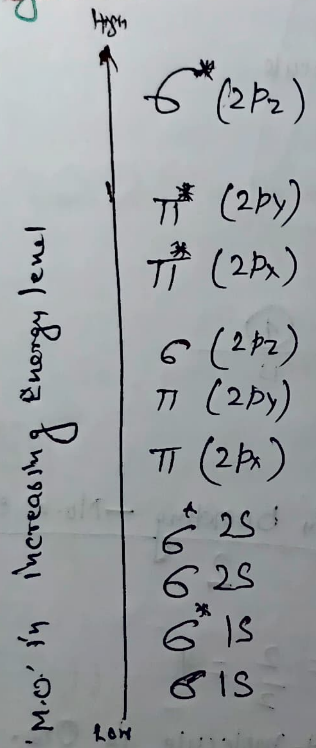
$\sigma(2p_z)\pi^* 2p_x, \pi^* 2p_y\ \sigma^* 2p_z$

* denotes antibonding Molecular orbitals.

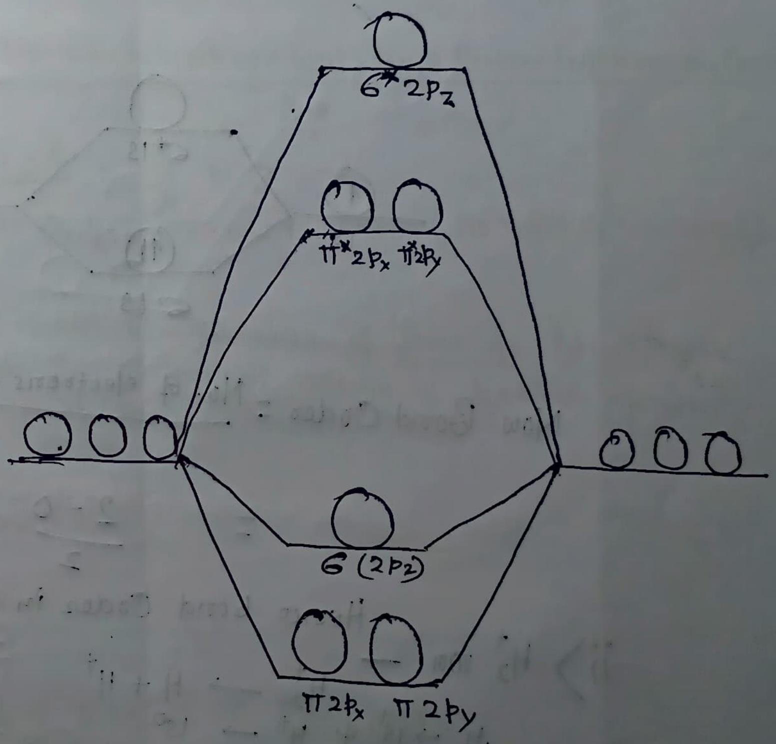
When we are writing molecular orbital configuration Hund's rule is obey i.e Hund's rule is always obeyed when we are writing M.O configuration

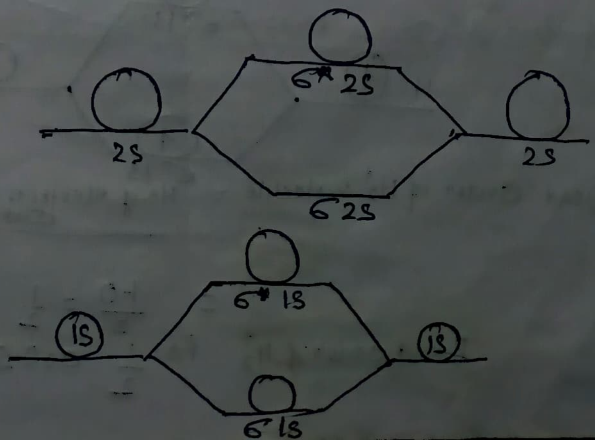
$KK\ \sigma(1s)\ \sigma^*(1s)\ \sigma(2s)\ \sigma^*(2s)\ \pi(2p_x)\ \pi(2p_y)\ \sigma(2p_z)$ ----- $\pi^*(2p_x)\ \pi^*(2p_y)\sigma^*(2p_z)$

[Highest the bond Order value Shortest is the Bond-length value.]



Representation chart of M.O. diagram.





Molecular Orbital Configuration of A_2 type.

(i) H_2 (ii) H_2^+

i.e. species having only σ_s & σ^*_s Molecular orbital.

1) M.O Configuration of H_2 and M.O diagram of H_2 and bond order in H_2 molecule.

$H_2 = H + H$

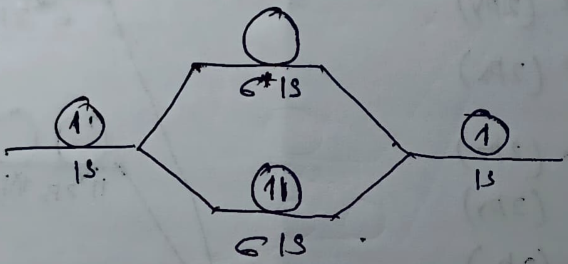
$_1H + {}_1H = H_2$

Total Number of electron in H_2 Molecule = 2

So, molecular Configuration will be

$\sigma 1s^2 \sigma^* 1s^0$

M.O Diagram of H_2 molecule



Now Bond Order = $\frac{\text{No. of electrons in bonding} - \text{No. of electrons in Anti bonding}}{2}$

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

Hence bond Order in H_2 molecule is One.

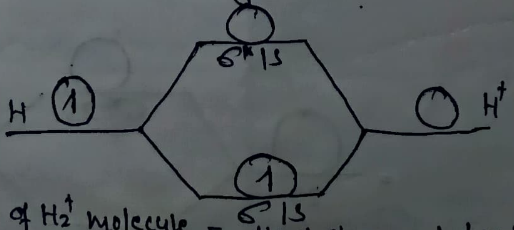
ii) H_2^+ ion: —

$H_2^+ \longrightarrow H + H^+$

$_1H \to 1s^1$ & $H^+ \to 1s^0$

The total number of electron in H_2^+ molecule = 1+0 = 1

Now Molecular Obital Configuration → $\sigma 1s^1 \sigma^* 1s^0$



Bond Order of H_2^+ molecule = $\frac{\text{No of electron in bonding Orbital} - \text{No of electron in Anti bonding Orbital}}{2}$

$= \frac{1-0}{2} = \frac{1}{2} = .5$

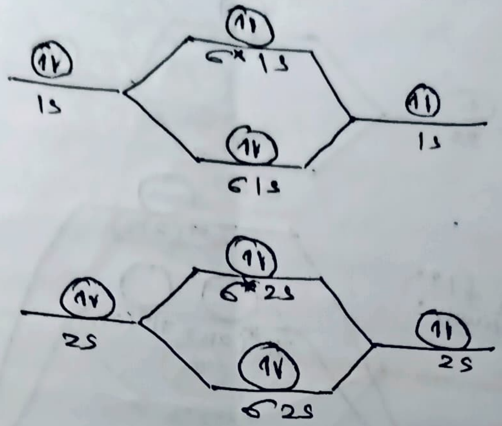
Bond order of H_2^+ is $\frac{1}{2}$ or 0.5

in Be_2 molecule = 4+4 = 8

Orbital Configuration

$\sigma 1s^2 \ \sigma^* 1s^2 \ \sigma 2s^2 \ \sigma^* 2s^2$

Mo. Diagram.



Bond order = $\frac{\text{No. of Electrons in bonding Orbital} - \text{No. of Electrons in Antibonding Orbital}}{2}$

$= \frac{4-4}{2} = \frac{0}{2} = 0$

So, Bond Order in Be_2 Molecule is Zero. (No bond is established)

Type Ⓑ :- Molecular Orbital Configuration of some A_2 type specific compound in which two identical atoms of p-block elements of second period of Modern Periodic Table.

(i) B_2 (Molecule)

$_5B \rightarrow 1s^2 \ 2s^2 \ p^1$ $\square$ 1s

$B_2 \rightarrow B+B = 5+5 = 10$ Electrons

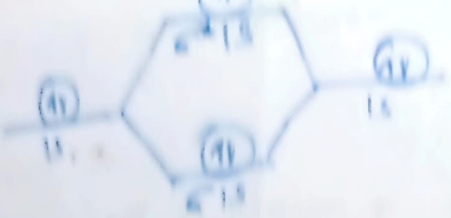
∴ Total number of electrons in B_2 molecule = 10

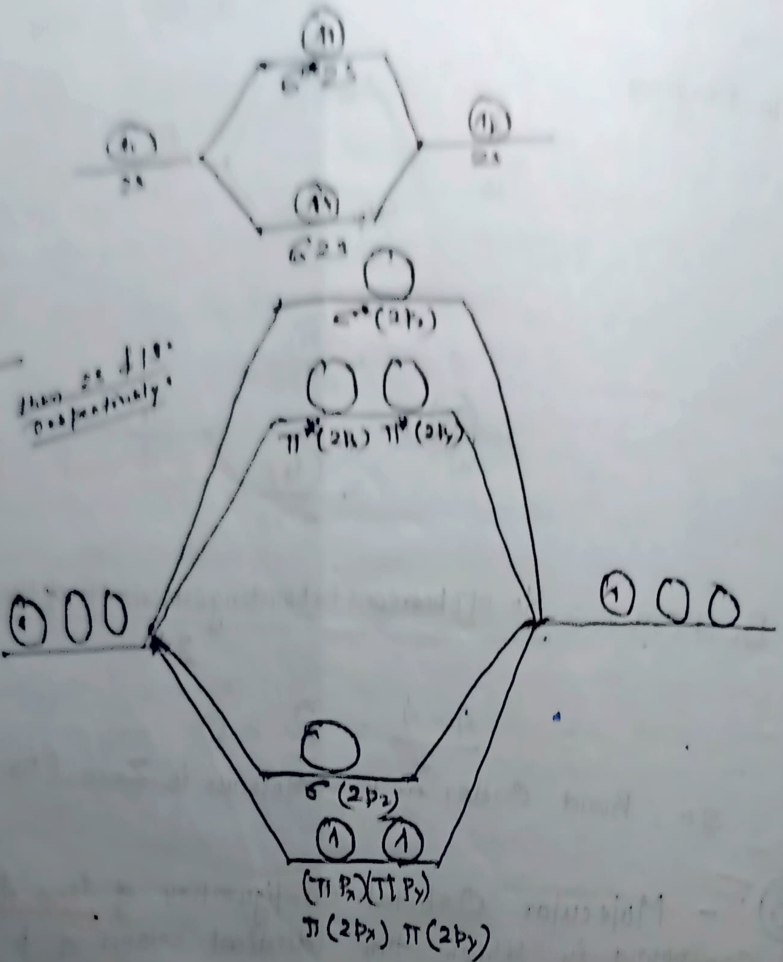
Molecular Orbital Configuration of B_2 molecule

$\sigma 1s^2 \ \sigma^* 1s^2 \ \sigma 2s^2 \ \sigma^* 2s^2 \ \pi (2p_x)^1 \ \pi (2p_y)^1 \ \sigma 2p_z^0$

[According to Hund's rule]

P.T.O





Now Bond Order $= \dfrac{\text{No. of electron in bonding Orbital} - \text{No. of electron in antibonding Orbital}}{2}$

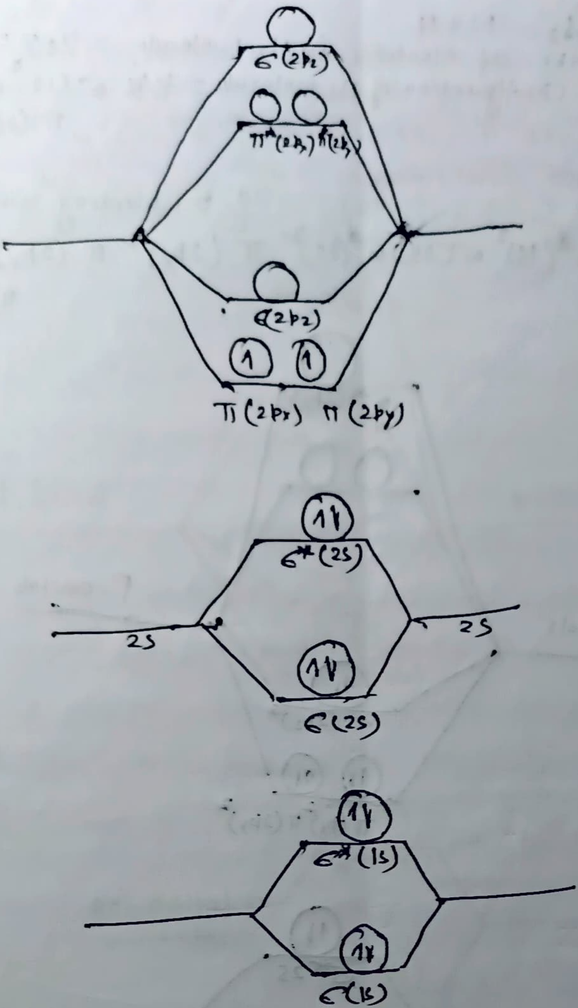
$$= \frac{06 - 04}{2} = \frac{2}{2} = 1$$

So, bond order is one.

<u>Note</u>

If bond order increases the bond length decreases.

Representation of M.O diagram of B_2 as follow



$$\text{Bond Order} = \frac{\text{No. of Total Electrons in bonding Orbital} - \text{No of Total electro antibonding O}}{2}$$

$$= \frac{6-4}{2} = \frac{2}{2} = 1$$

the bond Order in B_2 molecule $= 01$