Molecular Orbital Configuration

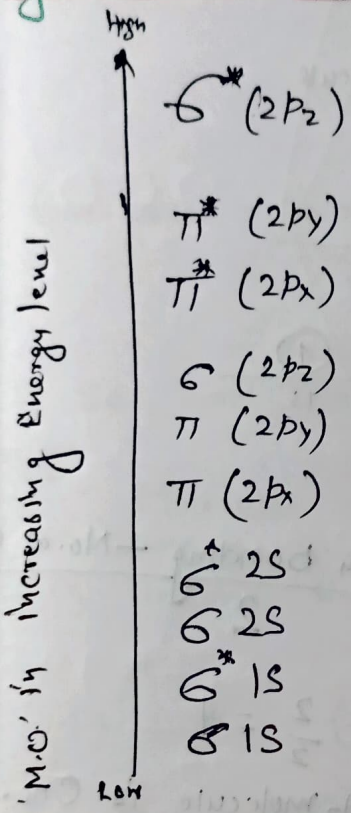
$\sigma 1s, \sigma^* 1s, \sigma 2s, \sigma^* 2s, \pi(2p_x)\ \pi(2p_y)$

* denotes antibonding Molecular orbitals. $\sigma(2p_z)\ \pi^* 2p_x, \pi^* 2p_y\ \sigma^* 2p_z$

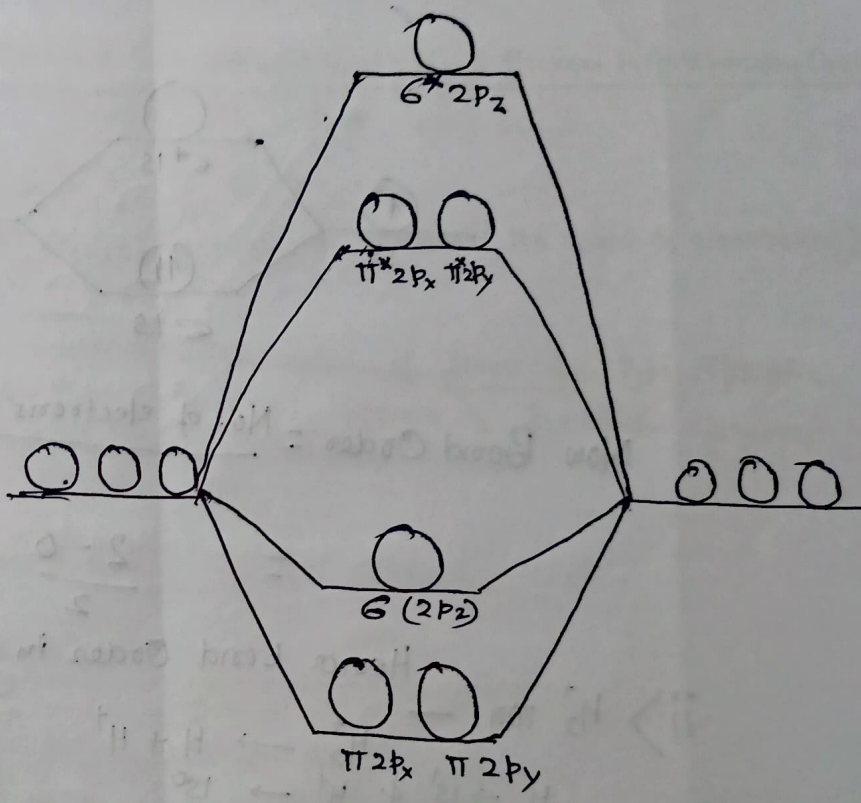
When we are writing molecular Orbital Configuration Hund's rule i.e Hund's rule is always obeyed when we are writing M.O configuration

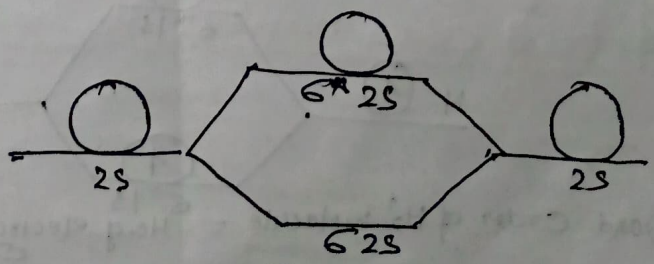
$KK\ \sigma(1s)\ \sigma^*(1s)\ \sigma(2s)\ \sigma^*(2s)\ \pi(2p_x)\ \pi(2p_y)\ \sigma(2p_z) \ldots\ \pi^*(2p_x)\ \pi^*(2p_y)\ \sigma^*(2p_z)$

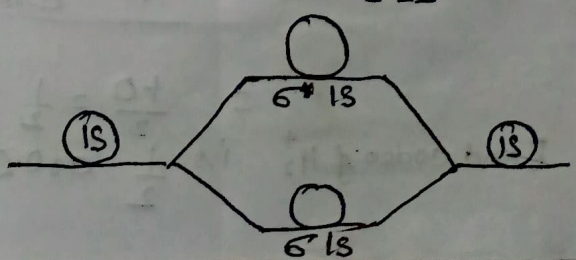
[Highest the bond Order value Shortest is the Bond length value.]



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.

$H_2 = H + H$

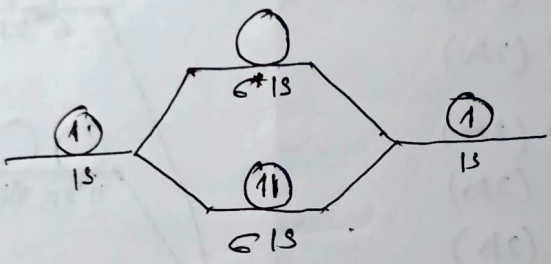
$_1H + _1H = H_2$

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 = $\frac{\text{No. of electrons in bonding} - \text{No. of electrons in antibonding}}{2}$

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

Hence bond Order in H_2 molecule is One.

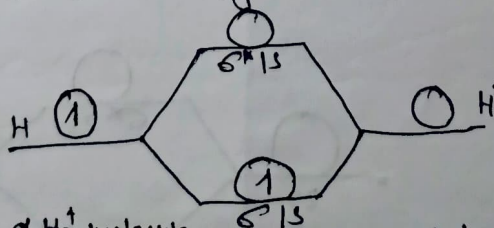
ii) H_2^+ ion :—

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

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

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

Now Molecular Orbital Configuration. → $\sigma 1s^1 \; \sigma^* 1s^0$



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

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

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