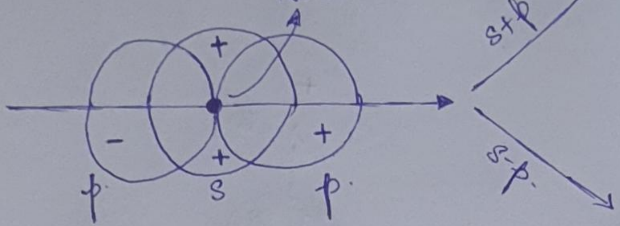
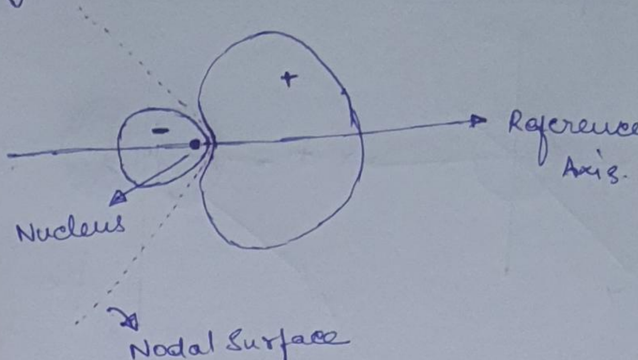
CH1101 Assignment -7

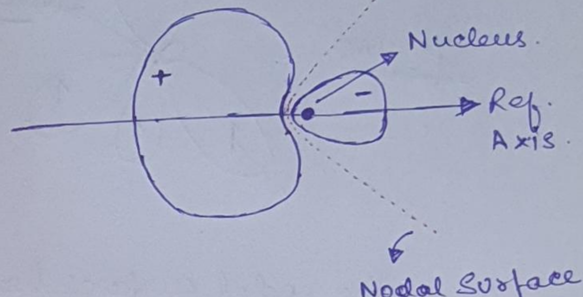
Name: Priyanshu Mahato

Roll No.: pm21m002.

Q1. **sp Orbital** :-

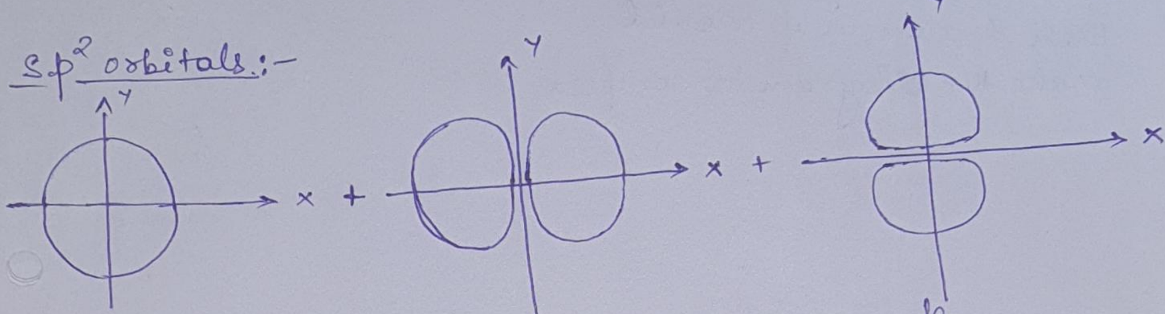


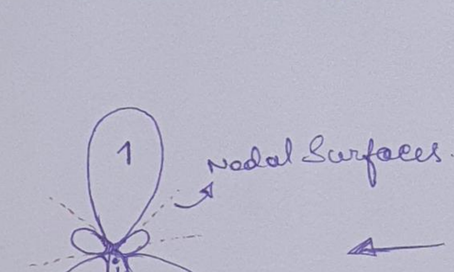




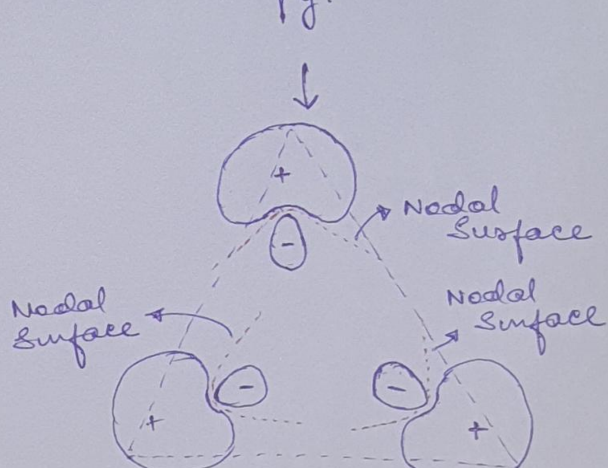
(Reference axis is the axis along which the p-orbital is oriented)

sp^2 orbitals :-



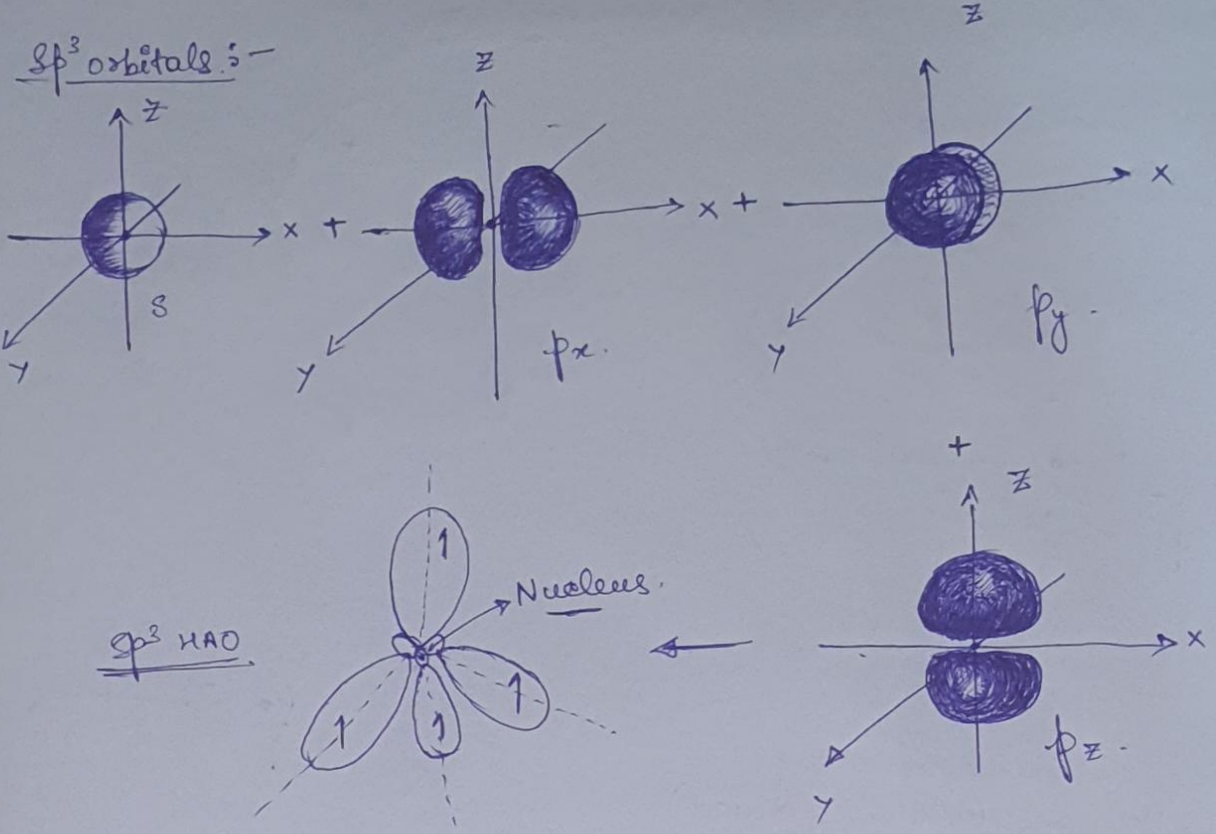


sp^2 HAO.



sp^2 hybrid orbitals.

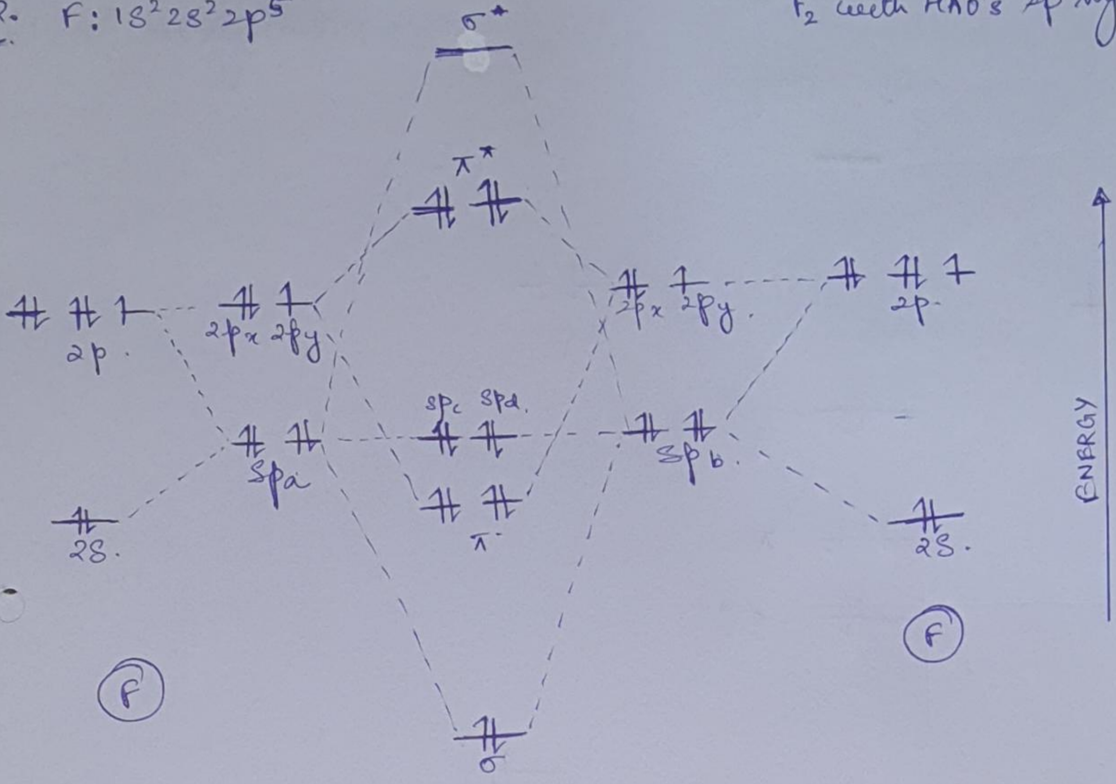
sp^3 orbitals :-



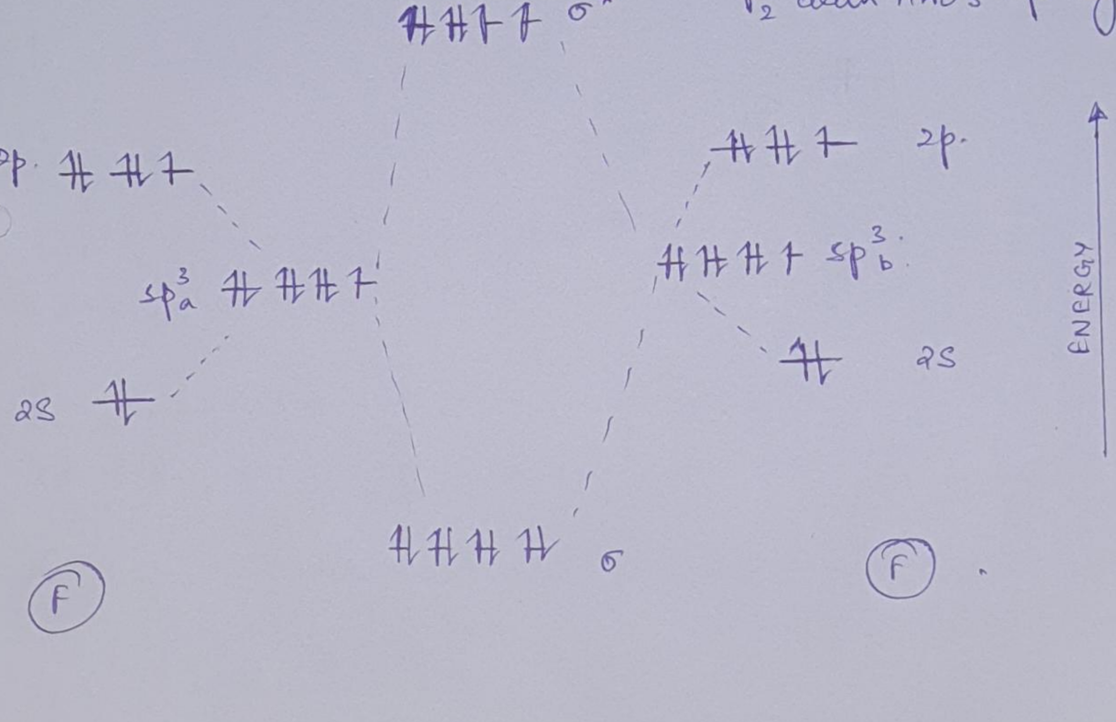
The nodal surfaces haven't been drawn, as it would make the diagram too complex.

Q2. F : $1s^2 2s^2 2p^5$

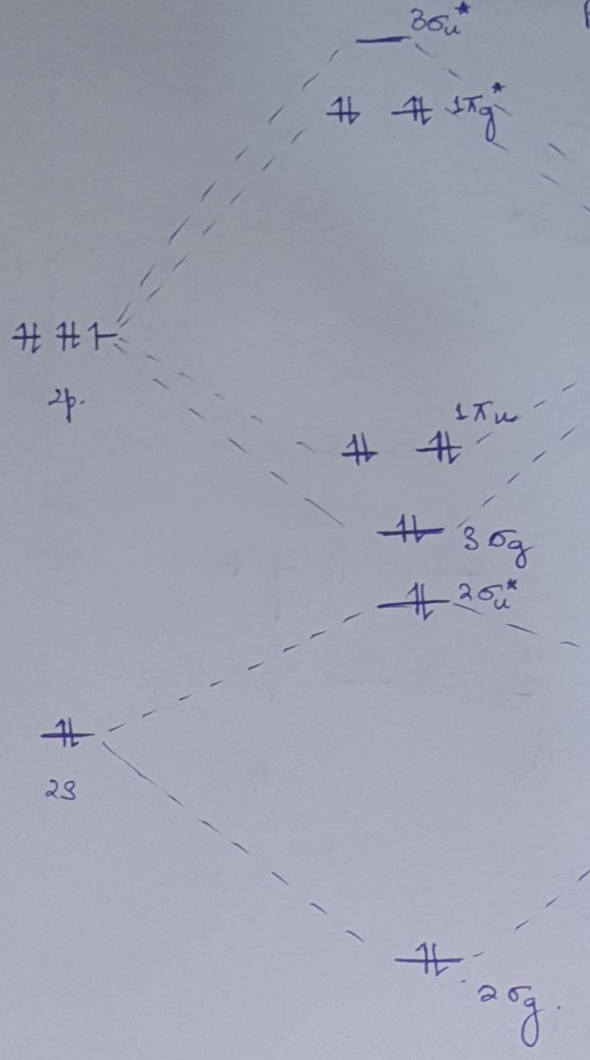
F_2 with HAO's sp hybridised



F_2 with HAO's sp^3 hybridised



Full MO diagram for F_2.

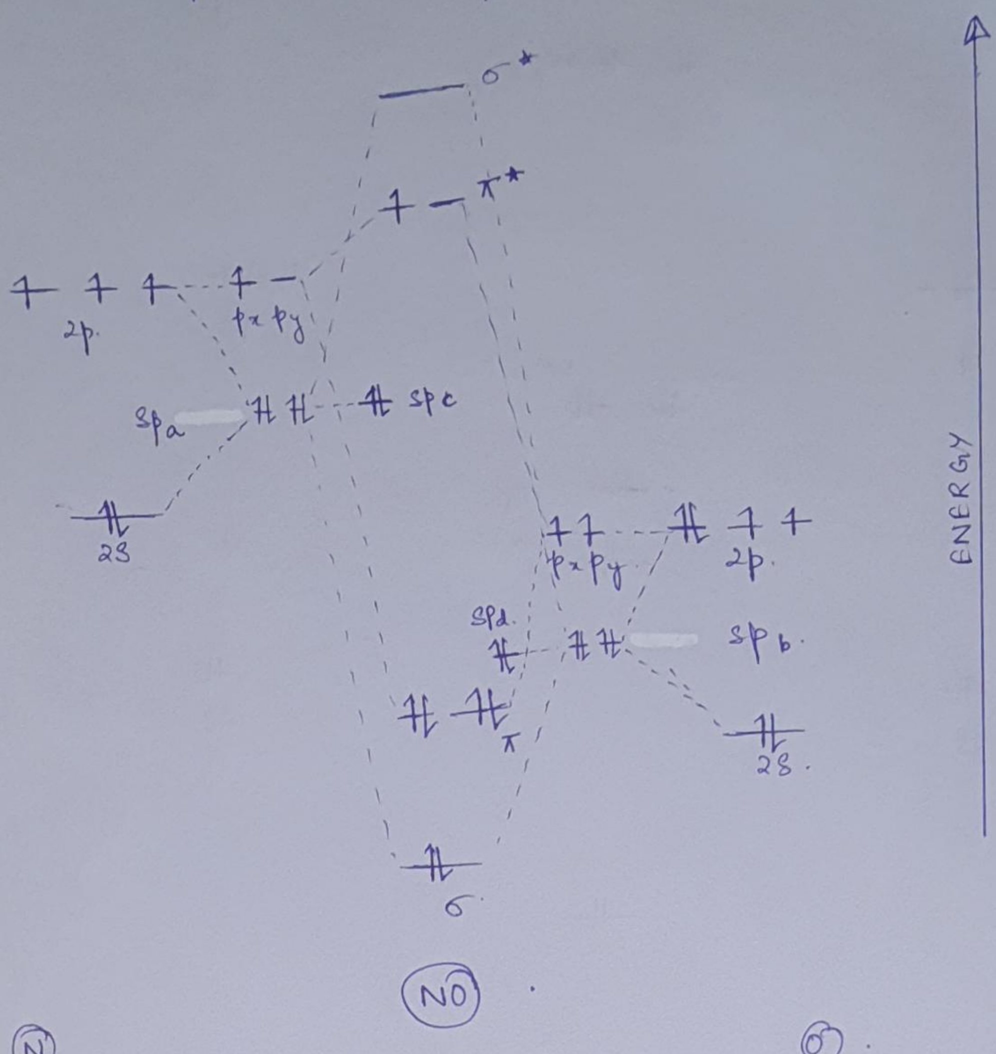


In sp hybridisation, σ, π and π^* are fully occupied and σ^* is empty so, $BO = \frac{6-4}{2} = 1$

In sp^3 hybridisation, σ is fully occupied and in σ^* has 2 less than fully occupied orbitals, $BO = \frac{8-6}{2} = 1$.

In the full MO diagrams, all the 3 BO's are fully occupied and ABO's are 2 electrons short than fully filled. i.e., $BO = 1$, again.

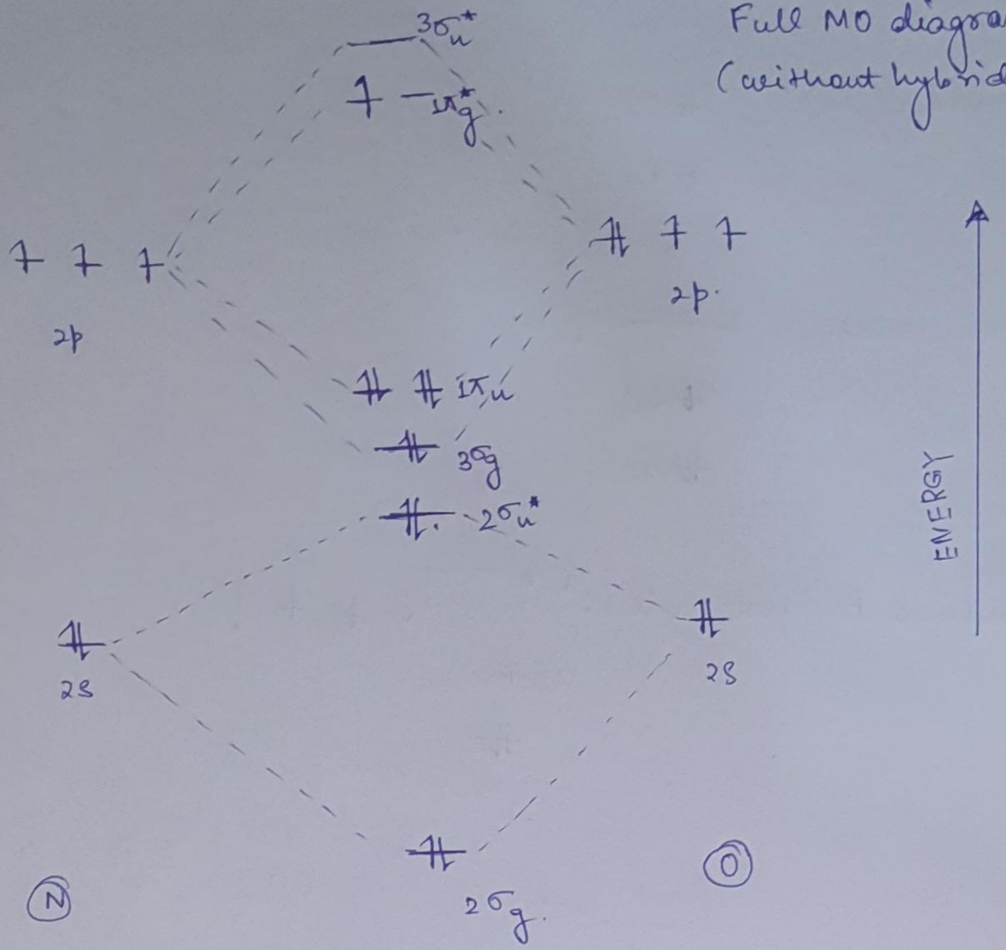
Q3. N: $1s^2 2s^2 2p^3$; O: $1s^2 2s^2 2p^4$



Considering both N and O to be sp hybridised, the π* orbital is the HOMO and it is not completely filled. The σ* is the LUMO. The σ, π and π* are fully filled orbitals, and there are two lone-pairs of electrons which are sp hybrised.

$$B.O. = \frac{6-1}{5} = \underline{2.5}$$, which matches the literature value.

Full MO diagram for NO
(without hybridisation)



Comparing the hybridised and non-hybridised MO's, we find that the MO with non-HAO's doesn't predict the existence of non-bonding (lone pairs) electrons, as observed experimentally. The MO with HAO's not only tells us about the existence of lone pairs of electrons but it also explains the hybridisation and degeneracy of the non-bonding electrons.

<u>NOTE</u>: Experimental and computational data show that sp mixing does occur in NO although theoretically it shouldn't. Therefore, in the above MO, $1\pi_u$ should be lower in energy than $3\sigma_g$ (experimentally).

Q4. (a) $1s^2 2s^2$.

Be (Ground State): $\uparrow\downarrow$ 2s

$\uparrow\downarrow$ 1s

Be (Excited state): $\uparrow$ — — 2p

$\uparrow$ 2s

$\uparrow\downarrow$ 1s

Be (Hybridised Excited State): 2p $\uparrow$ p_z — p_x — p_y $\uparrow$ $\uparrow$ sp

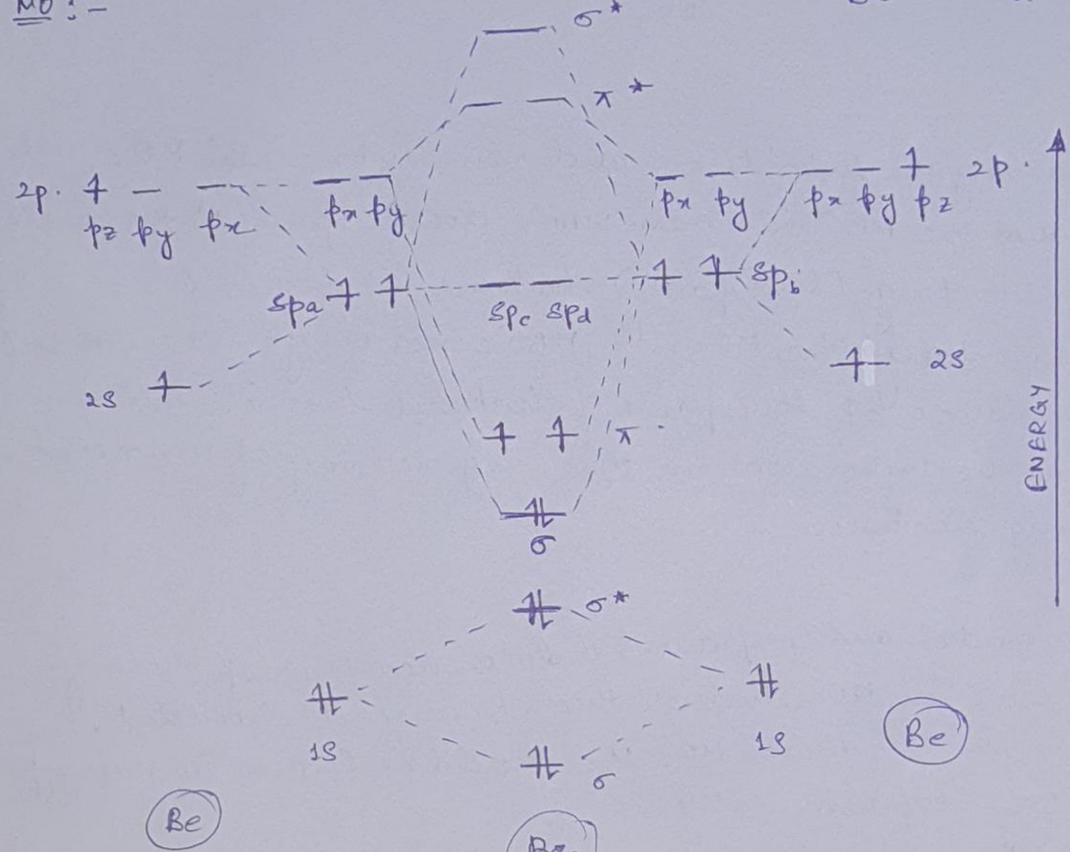
2s $\uparrow$

$\uparrow\downarrow$

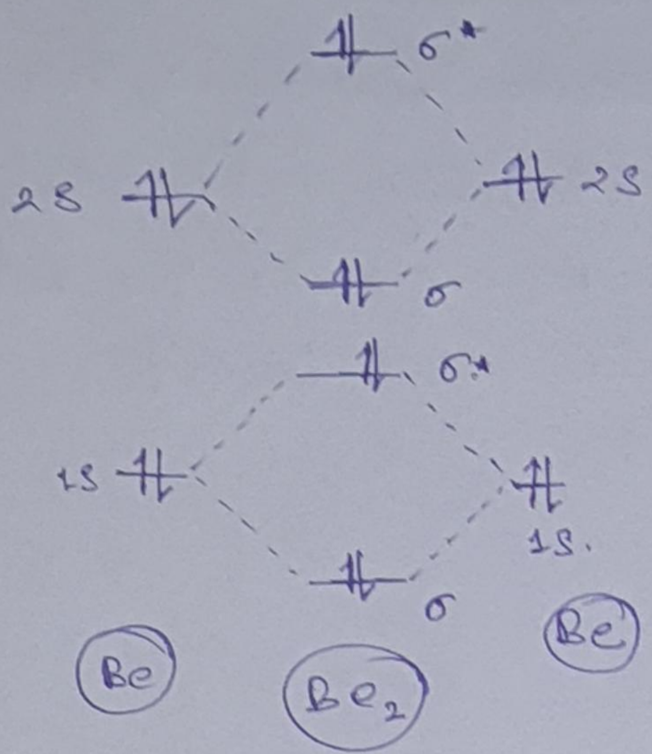
1s

MO :-

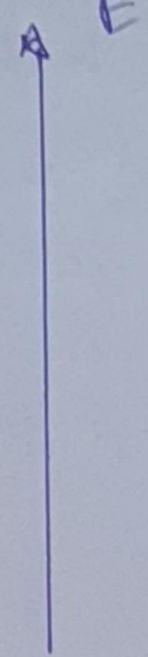
$$BO = \frac{6-2}{2} = \frac{4}{2} = 2.$$



Considering normal MO,



BO = $\underline{\underline{0}}$.



while considering the sp hybridisation, the BO is 2, which is greater than in the normal MO, for which BO = 0.

When we consider sp hybridisation, σ formed by sp HAO's is lower in energy than σ_{2s}, thus, making it a more stable system (lower energy $\Leftrightarrow$ stable system), therefore, allowing the formation of weak bonds as opposed to no bond formation in normal MO's as BO = 0.

(b) Li_2 $BO = \frac{4-2}{2} = 1$

In Li_2, the BO is 1, therefore, here, bonds exist, but in Be_2, $BO=0$, so here, the molecule (and hence, bonds) doesn't exist. However, exceptionally, when we consider s-p hybridisation, the BO increases to 2 and it allows the formation of some weak bonds.