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ROLL NO. : pm21ms002

Q1. a) $R_H = 13.6$, BE (2p) $= -349.7$ eV

$$E_n = \frac{-Z_{eff}^2 R_H}{n^2} \Rightarrow Z_{eff} = \sqrt{\frac{-E_n \cdot n^2}{R_H}} = \sqrt{\frac{-(-349.7) \times 4}{13.6}}$$

$\therefore$ $\boxed{Z_{eff} = 10.142.}$ ans.

b) Radial part of 2s AO Ψ,

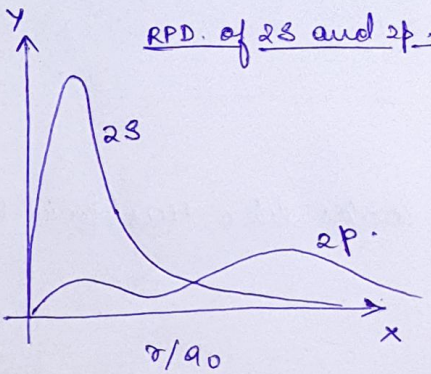
$$\left(\frac{1}{2a_0}\right)^{3/2} \left(2 - \frac{r}{a_0}\right) e^{\frac{-r}{2a_0}}$$

For finding positions of radial nodes,

$$\left(\frac{1}{2a_0}\right)^{3/2} \left(2 - \frac{r}{a_0}\right) e^{\frac{-r}{2a_0}} = 0.$$

$$\Rightarrow 2 - \frac{r}{a_0} = 0 \Rightarrow \frac{r}{a_0} = 2 \Rightarrow \boxed{r = 2a_0} \text{ ans.}$$

c) RPD of 2s and 2p.



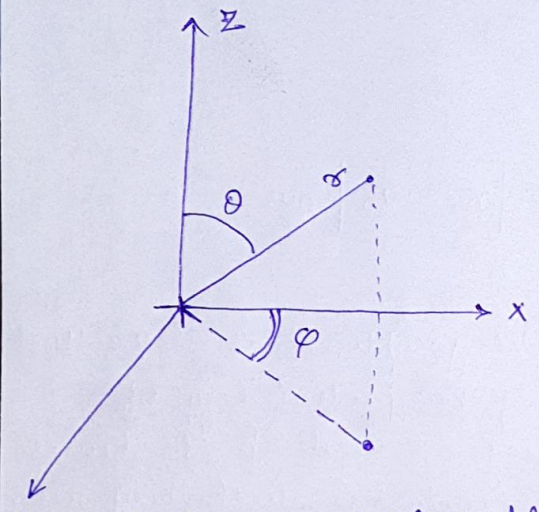
From the graph, it is clear that most of the probability of finding 2s and 2p electrons lies outside the shielding area of 1s electrons. But 2s has a local maxima closer to the nucleus, most of which, lies inside the region occupied by 1s. This tells us that 1s doesn't shield 2s electrons completely. However, a very insignificant portion of 2p (the 'tail' of the RPD) lies in 1s region. Thus, 1s shields 2p electrons far better than it does in the case of 2s electrons.

We can thus say that 2s experiences greater effective nuclear charge due to the possibility of being inside the 1s screen, and 2p experiences much less effective nuclear charge. We can also deduce that the overall energy of 2s is lower than 2p (but $|E_{2s}| > |E_{2p}|$). Therefore, 2s can shield electrons better than 2p.

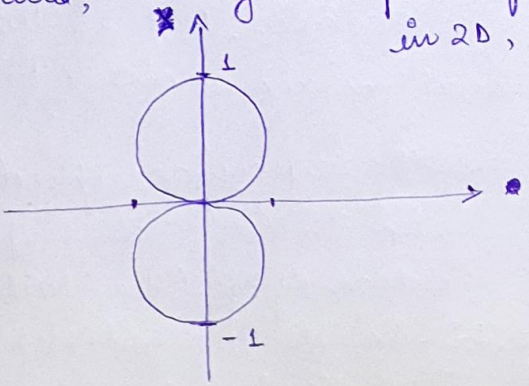
d) The diagram (1) best represents σ^* MO. This is because the contribution to the BMO is greater from the a AO which has lower energy and contribution to the ABMO is more from the AO at higher energy level.

Q2. Angular part of p_x orbital : $\sqrt{\frac{3}{4\pi}} \sin\theta \cos\varphi$

The 3-D cartesian coordinates look as follows:



and, the angular plots of $\sin x$ looks like this (from $[0, 2\pi]$), in 2D,



Here, the angle 'θ' is defined as the azimuthal angle. It is the angle made by Z axis and the st. line joining the origin and the point.

Now, 'φ' is defined as the colatitude angle. It is the angle between the projection of 'r' on the XY plane and the X-axis.

The Nodal plane corresponds to the region where the angular part of the wavefunction becomes zero (0).

$$\Rightarrow \sqrt{\frac{3}{4\pi}} \sin\theta \cos\phi = 0$$

$$\Rightarrow \sin\theta \cos\phi = 0$$

This can be possible in 3 cases.

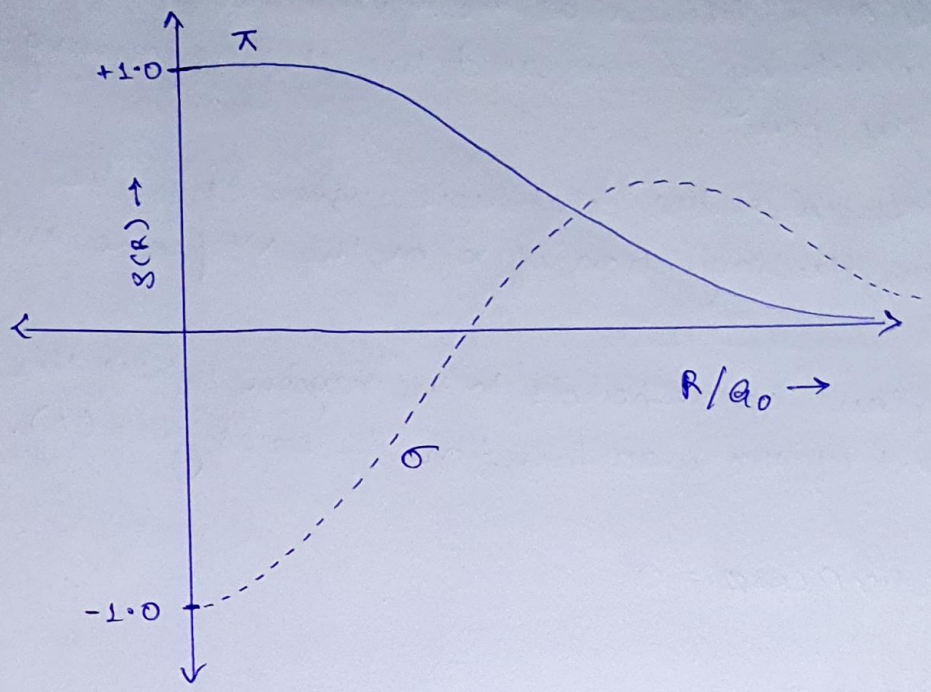
(i) $\sin\theta = 0$

(ii) $\cos\phi = 0$, or,

(iii) $\sin\theta = 0$ and $\cos\phi = 0$ ← This is the feasible case for a nodal plane.

$$\therefore \boxed{\theta = 0 \text{ and } \phi = \frac{\pi}{2}} \text{ ans.}$$

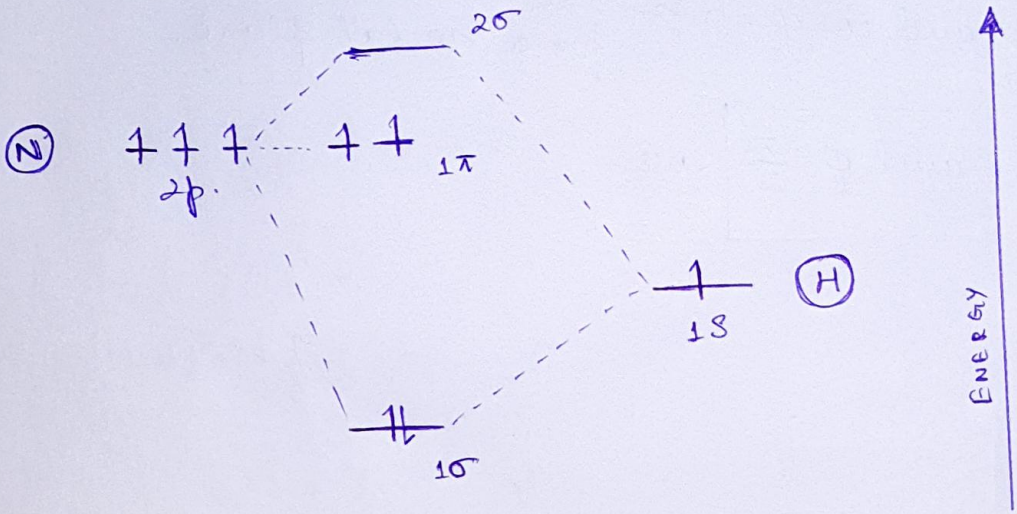
Q3.

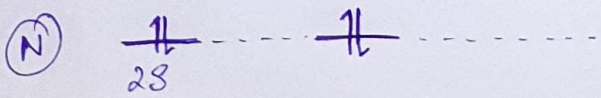


Q4. NH.

(A). H(1S) = -13·6 eV ; N(2S) = -25·6 eV

N(2p) = -13·2 eV





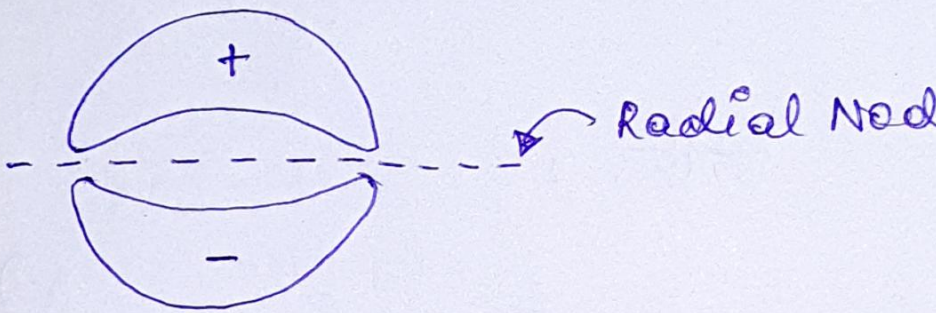
B) Just like O_2, there would be 3 possible spin states in NH too,

For 1π, (i) $\uparrow\uparrow$ (ii) $\uparrow\downarrow$ (iii) $\uparrow\ \uparrow$

Out of these, (i) would serve as the <u>Ground State</u> as it has minimum energy $\Leftrightarrow$ maximum stability.

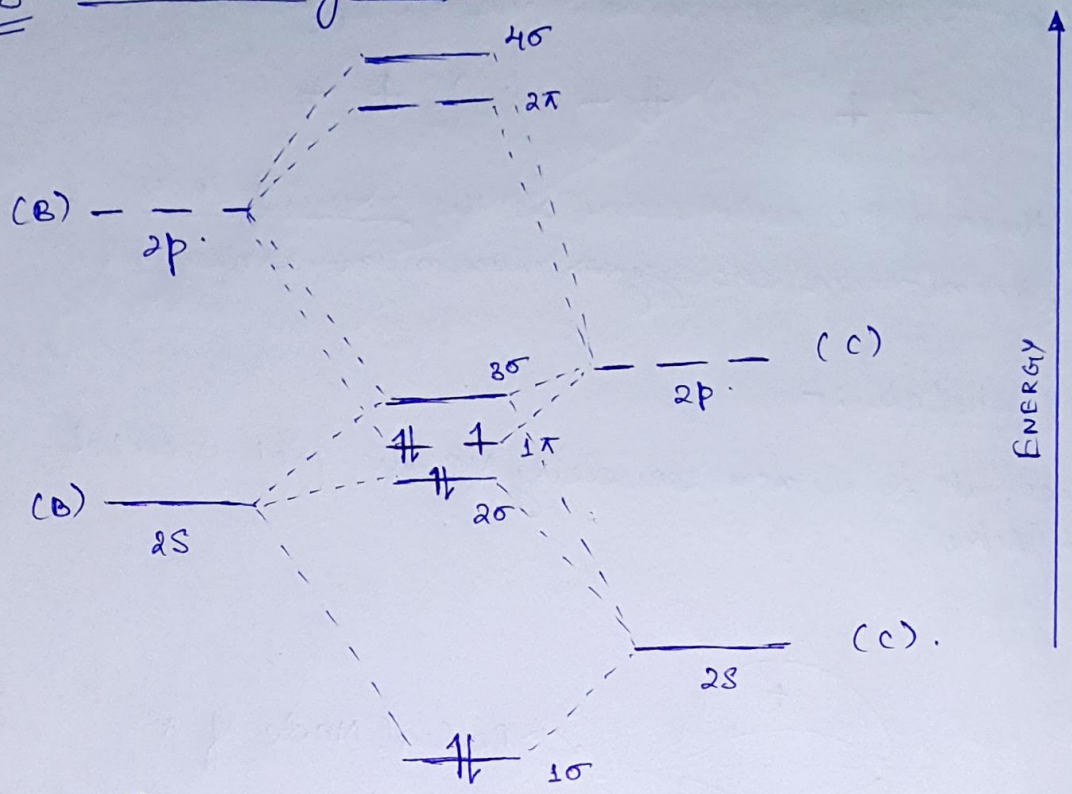
(c) <u>π MO sketch</u> :-

- Since, it is a non-bonding MO, the plot would look like,



(a)

Qs. BC MO-diagram :-



(B)

(B) for BC : $1\sigma^2$

for BC^{1-} : $1\sigma^2$

(C).

(B) for BC : $1\sigma^2 1\sigma^{*2}\ 2\sigma^2 2\sigma^{*2}\ 1\pi_x^2\ 1\pi_y^2$.

for BC^{1-} : $1\sigma^2 1\sigma^{*2} 2\sigma^2 2\sigma^{*2}\ 1\pi_x^2\ 1\pi_y^2$.

} Includes MO for 1s orbital too, which hasn't been considered in part (A).

(c) The BO of BC = $\frac{7-4}{2} = 1.5$

The BO of BC^{1-} = $\frac{8-4}{2} = 2$

As we know, if BO increases, bond length decreases, So, the B-C bond in BC^{1-} is smaller than BC.

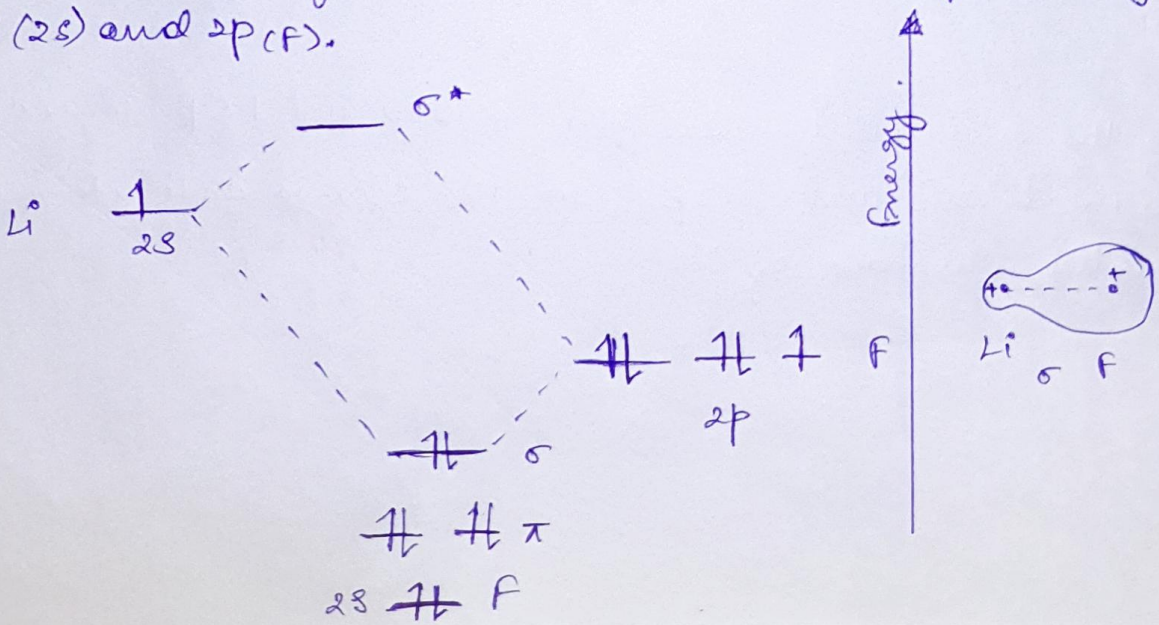
∴, B-C bond is stronger in BC^{1-}.

●

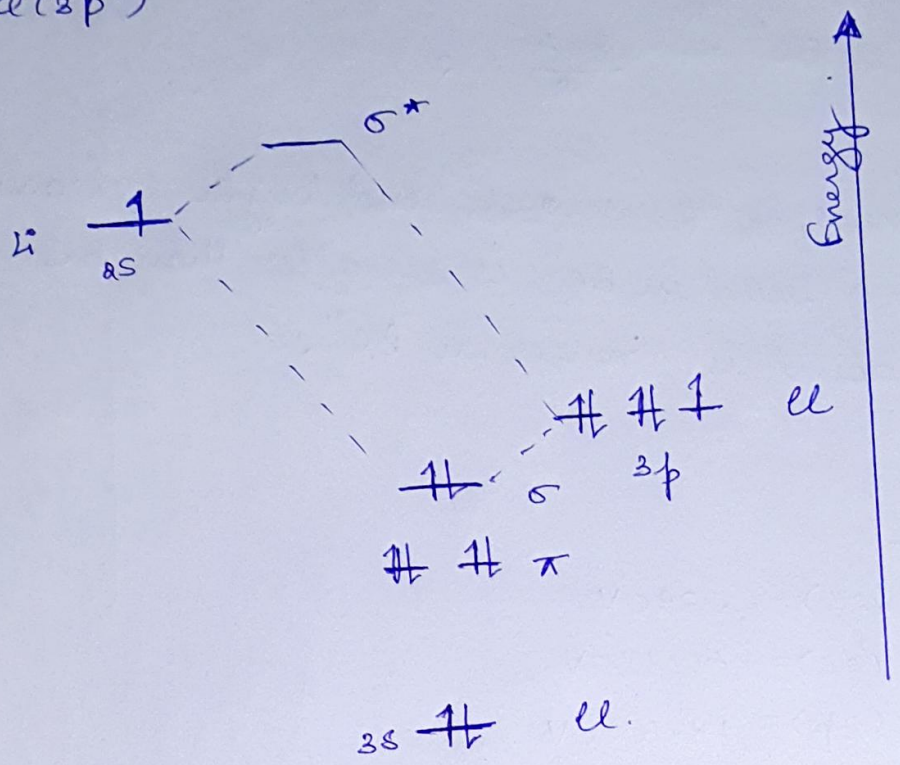
Q6. Energies :-

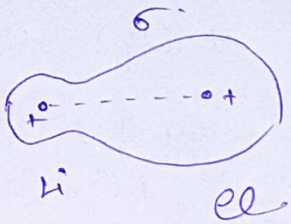
- Li (2S) = -5.39 eV
- F (2S) = -40.17 eV
- F (2p) = -18.65 eV
- Cl (3S) = -25.23 eV
- Cl (3p) = -13.67 eV

● As the energy of Li (2S) is closer to energy of 2p of F than the 2S of F, the BO and ABO will be formed by Li (2S) and 2p (F).



As the energy of Li (2s) is closer to energy of Cl (3p) than Cl (3s), the BO and ABO will be formed by Li (2s) and Cl (3p·)





As the energy difference b/w Li (2s) and F(2p) is more than Li(2s) and Cl(3p), so, the charge on Li atom is higher in case of LiF.