Q. What is bond-order ?

Soln. The number of bonds in a molecule is one-half of the difference of the number of electrons in the bonding molecular orbitals and the Number of electrons in the antibonding molecular orbitals

Mathematically,

$$\text{Bond-order} = \frac{\left(\begin{array}{c}\text{No. of electrons in}\\ \text{bonding orbitals}\end{array}\right) - \left(\begin{array}{c}\text{No. of electrons}\\ \text{in antibonding}\\ \text{orbitals}\end{array}\right)}{2}$$

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

* Properties of Bond-order:

(a) A molecule is stable if $N_b > N_a$

(b) A molecule is unstable if $N_b < N_a$

In the other hand ⟶
Bond order as determined by the above formulla is very helpful as it given the following valuable information.

(i) Stability of the Molecule / Ion

A molecule / ion is stable if $N_b > N_a$

(ii) Bond dissociation Energy: It depends upon the bond order. Greater the bond order greater the bond dissociation energy

(iii) Bond length : Bond-order is inversely propotional to the bond length. Higher the bond order, smaller the bond length.

(iv) Magnetic properties : The presence of unpaired electrons in Molecular-orbitals of a species makes it paramagnetic in Nature. Greater the number unpaired electrons, the more will be its paramagnetic character.

On the other hand - if there are no unpaired electrons in MOs the species will be dia-magnetic in Nature.

* * ——— * * ——— * * ——— *

⇒ Nature of the Bonding MO'S orbitals :

$\sigma 1s$, $\sigma 2s$, $\sigma 2p_x$, $\pi 2p_y$, $\pi 2p_z$

⇒ Nature of the Anti Bonding MO's orbitals :

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

⇒ Sequence of MO's for, H, He, Li, Be, B, N :

$\sigma 1s < \sigma^* 1s < \sigma 2s < \sigma^* 2s < \pi 2p_y = \pi 2p_z < \sigma 2p_x < \pi^* 2p_y$
$= \pi^* 2p_z < \sigma^* 2p_x$

Sequence of MO's orbitals for O, F, Ne :

$\sigma 1s < \sigma^* 1s < \sigma 2s < \sigma^* 2s < \sigma 2p_x < \pi 2p_y = \pi 2p_z$
$< \pi^* 2p_y = \pi^* 2p_z < \sigma^* 2p_x$

We know that,

Bond order $\propto$ Bond Strength $\propto$ Bond Stability $\propto \frac{1}{\text{Bond length}}$.

Q. Why there is no existence of He_2 But He_2^+ formed Explain this theorem ?

Soln: Electronic configuration of He

$He(2) \rightarrow 1s^2$

So the sequence of M.O. orbitals

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

In this condition, $B.O = \frac{N_b - N_a}{2}$

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

So there is no existence of He_2.

In the other hand —

the electronic configuration of He^+

$He_2^+ \rightarrow 1s^1$

So the sequence of M.O for He_2^+

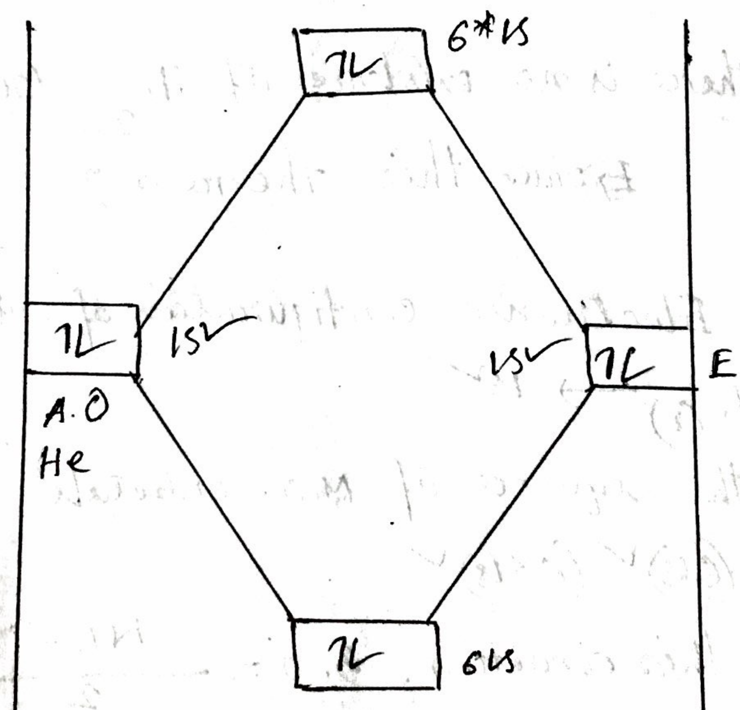
$(\sigma 1s)^2 (\sigma^* 1s^1)$

For this Bond-Order $= \frac{N_b - N_a}{2}$

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

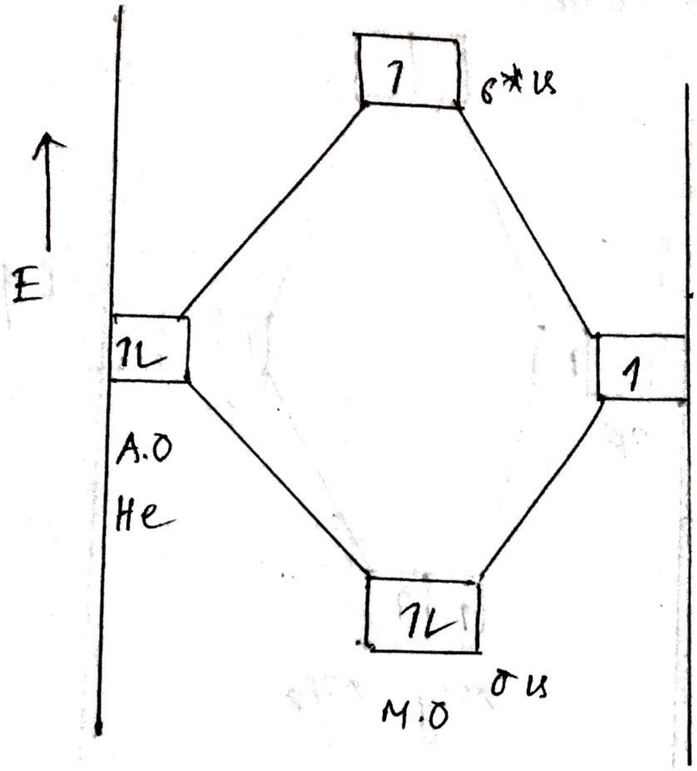
$= \frac{1}{2}$

Therefore the bond order is half So this ion is formed and stable.



M.O

He



Q, Describe the existence of B_2 and paramagnetic Nature of it?

Soln. Electronic Configuration of B atom

$B_{(5)} \longrightarrow 1s^2 2s^2 2p^1$

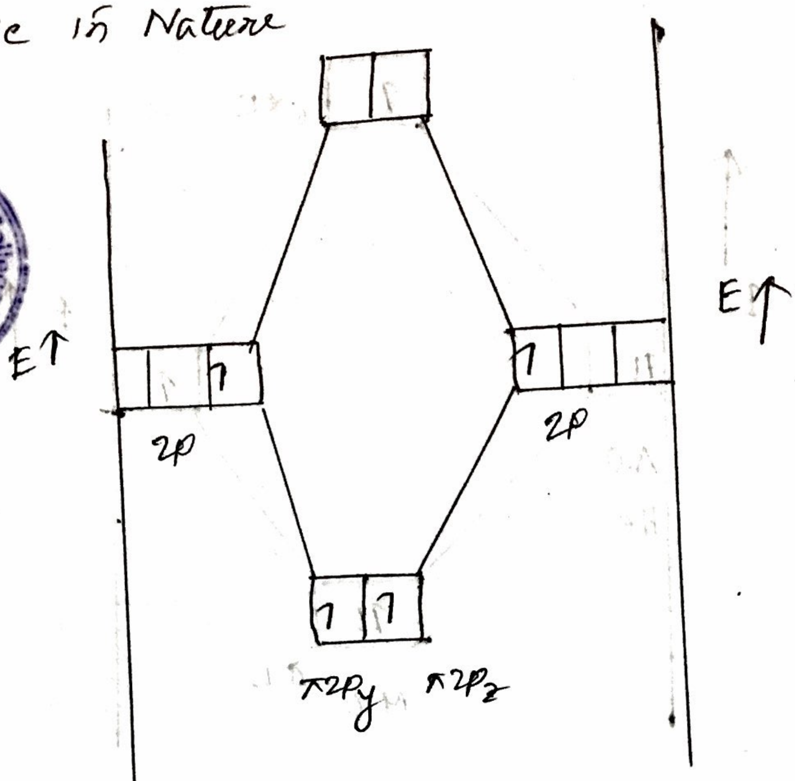
∴ Electronic configuration of B_2 Molecule :

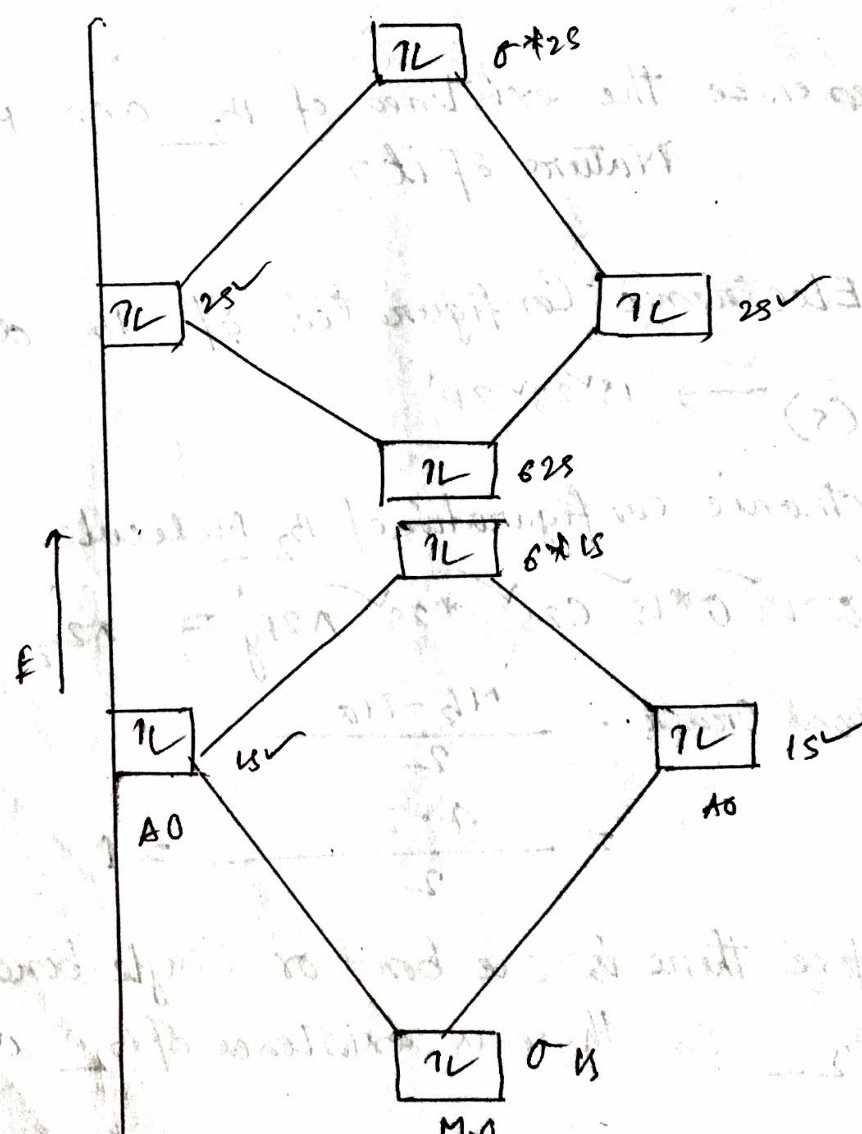
$\sigma 1s^2 \, \sigma^* 1s^2 \, \sigma 2s^2 \, \sigma^* 2s^2 \, \pi 2p_y^1 = \pi 2p_z^1$

$$\text{Bond Order} = \frac{N_b - N_a}{2}$$

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

Therefore there is one bond or Single bond in the B_2 So there is existence of B_2 and paramagnetic in Nature





Q. Describe the existence of C_2 and diamagnetic properties of it?

Soln. The electronic configuration of C atom

$1s^2 2s^2 2p_x^1 2p_y^1$

Total Number of electrons in C_2 Molecule

$= (6+6) = 12$

So the configuration of C_2 : $\sigma 1s^2 \sigma^* 1s^2$

$\sigma 2s^2 \sigma^* 2s^2 \pi 2p_y^2 = \pi 2p_z^2$

or, $KK \sigma 2s^2 \sigma^* 2s^2 \pi 2p_y^2 = \pi 2p_z^2$

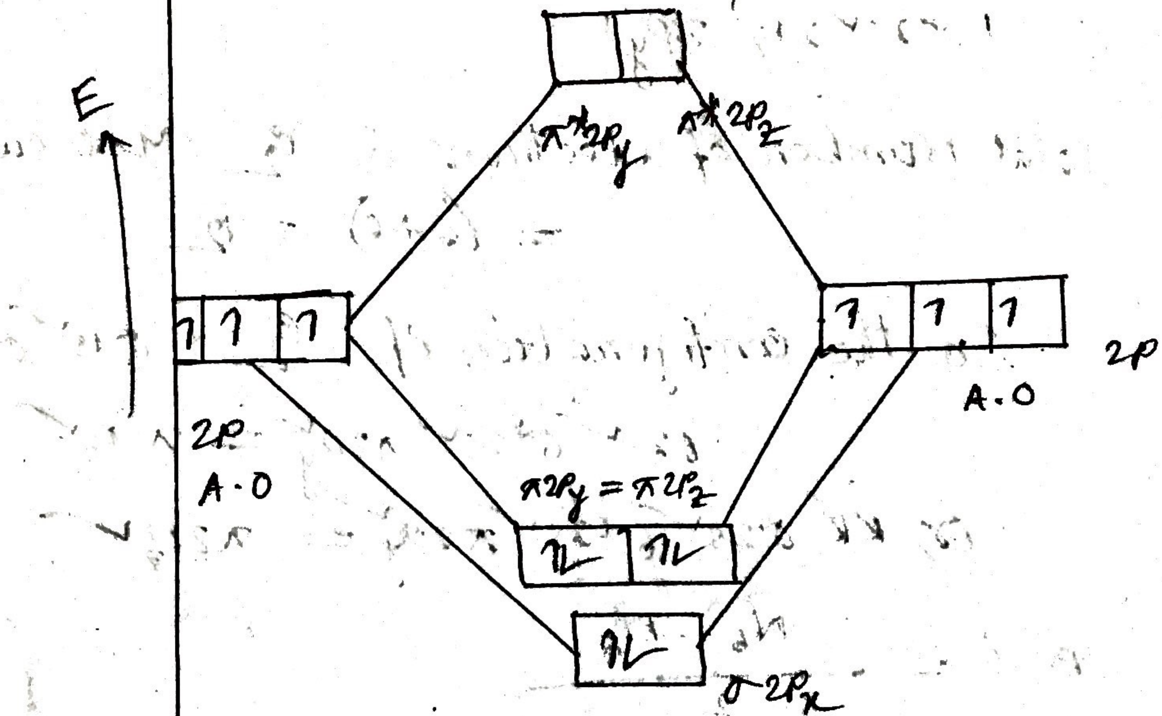
$$B.O = \frac{N_b - N_a}{2}$$

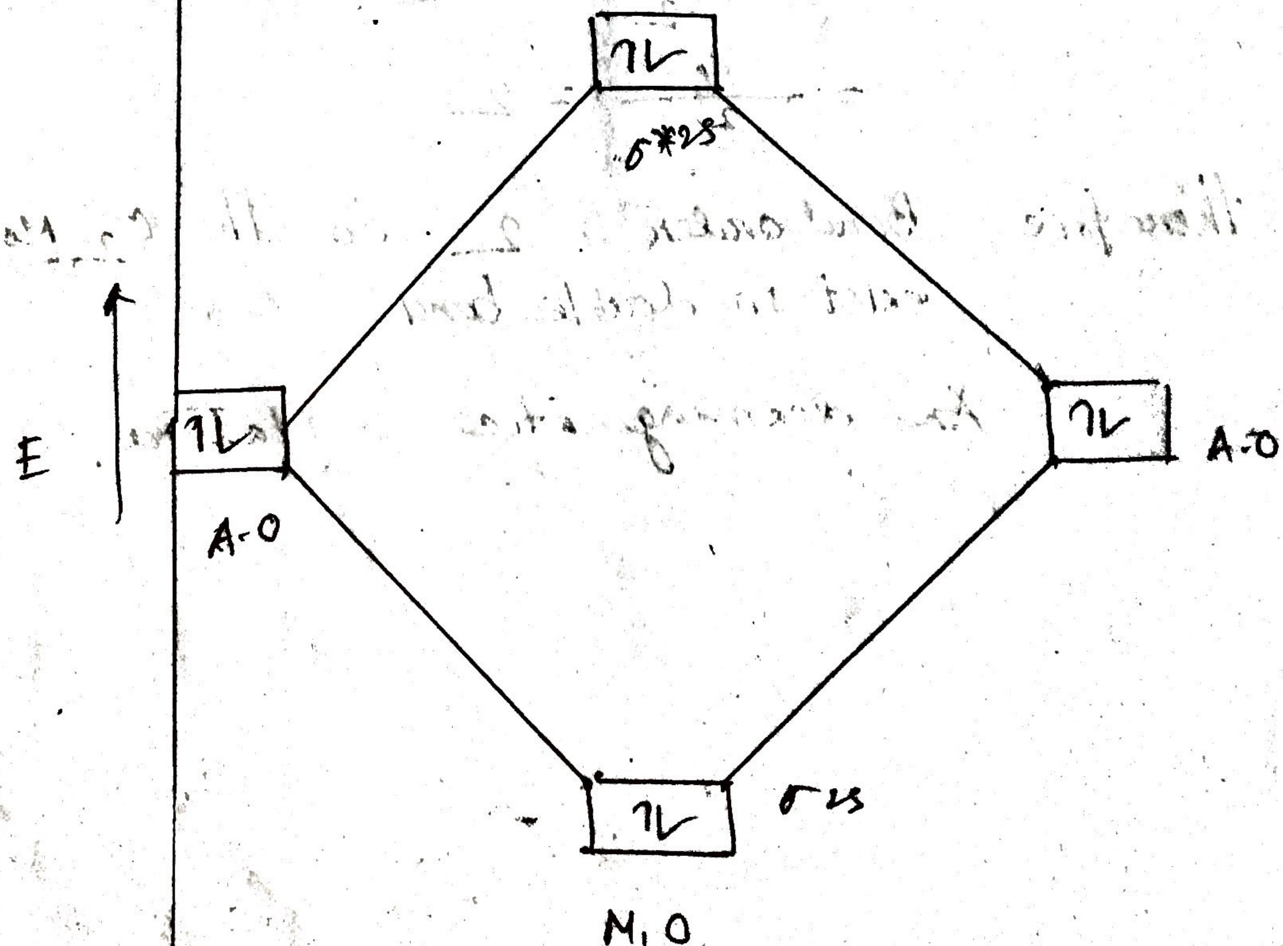
$$= \frac{6-2}{2}$$

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

therefore, Bond order is 2 So the C_2 Molecule exist in double bond

And diamagnetic in Nature.


E
π*2py
π*2pz
2p
A.O
2p
A.O
π2py = π2pz
σ2px


σ*2s
E
A.O
A.O
σ2s
M.O

Q. Describe the existence of O_2 and paramagnetic Properties of it?

Soln: The electronic configuration of O atom.

$O_{(8)} \longrightarrow 1s^2 2s^2 2p_x^2 2p_y^1 2p_z^1$

Total Number of electron in O_2 Molecule

$= (8+8) = 16$

Electronic Configuration of O_2 :

$\sigma 1s^2 \sigma^* 1s^2 \sigma 2s^2 \sigma^* 2s^2 \sigma 2p_x^2 \pi 2p_y^2 = \pi^2 2p_z \; \pi^* 2p_y^1$

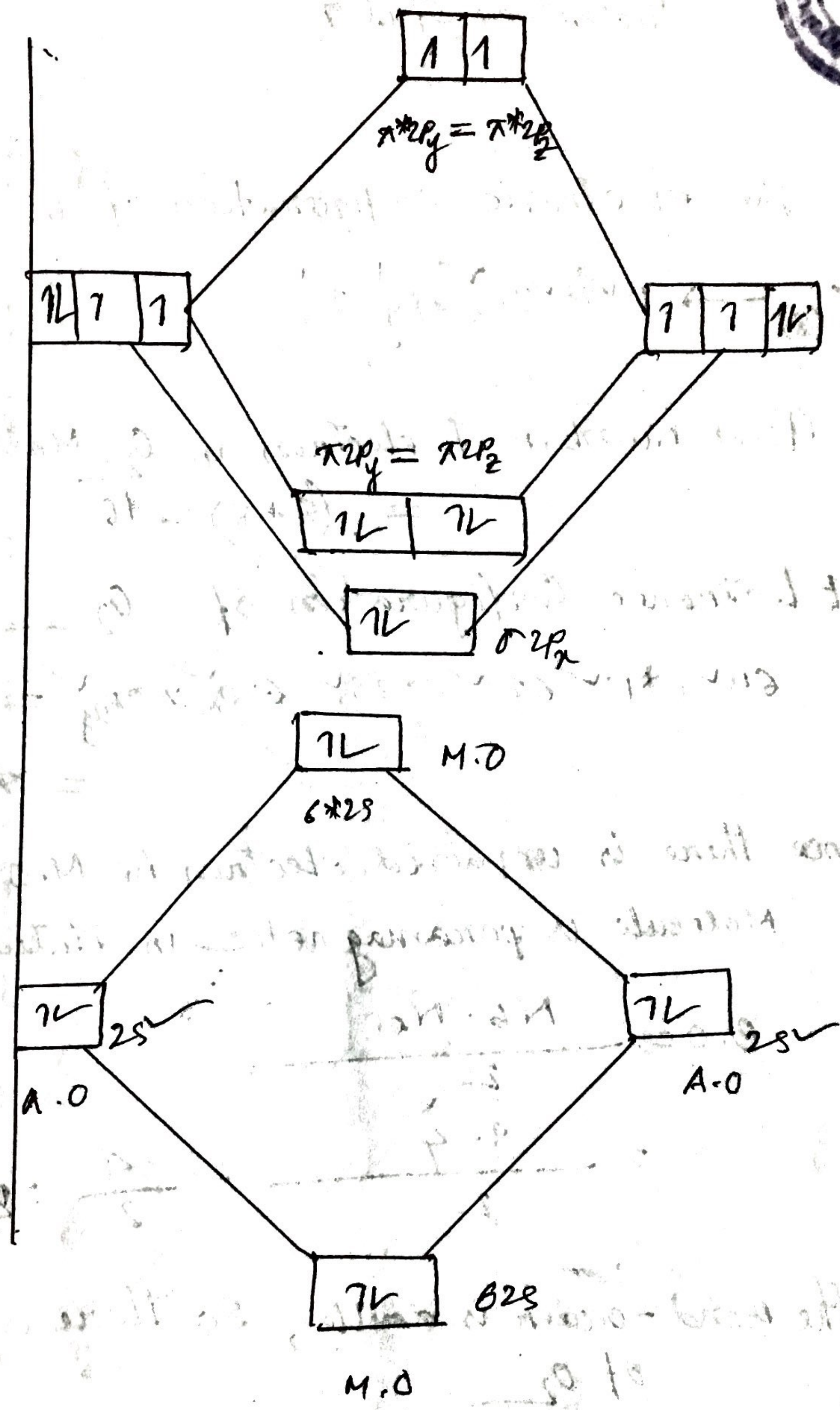
$= \pi^* 2p_z^1$

Hence there is unpaired electron in M.O. So O_2 Molecule is paramagnetic in Nature.

$$B.O = \frac{N_b - N_a}{2}$$

$$= \frac{8-4}{2} = \frac{4}{2} = 2$$

The Bond-order is double, So there is existence of O_2



O_2 - formation

Q. The Bond Strength of NO^+ is greater than that of NO ?

or,

In NO Molecule N–O bond length is greater than that of NO^+ ?

<u>Soln</u>. In NO molecule total Number of electron

$= (7+8) = 15$

So the electronic configuration of NO (15) :

$\sigma 1s^2\, \sigma^* 1s^2\, \sigma 2s^2\, \sigma^* 2s^2\, \sigma 2p_x^2\, \pi 2p_y^2 = \pi 2p_z^2$

$= \pi^* 2p_y^1 = \pi^* 2p_z^0$

$$B.O = \frac{N_b - N_a}{2}$$

$$= \frac{8-3}{2}$$

$$= \frac{5}{2} = 2.5$$

Again in NO^+ ion there are one electron less than NO

So the total Number of electron in NO^+ (14)

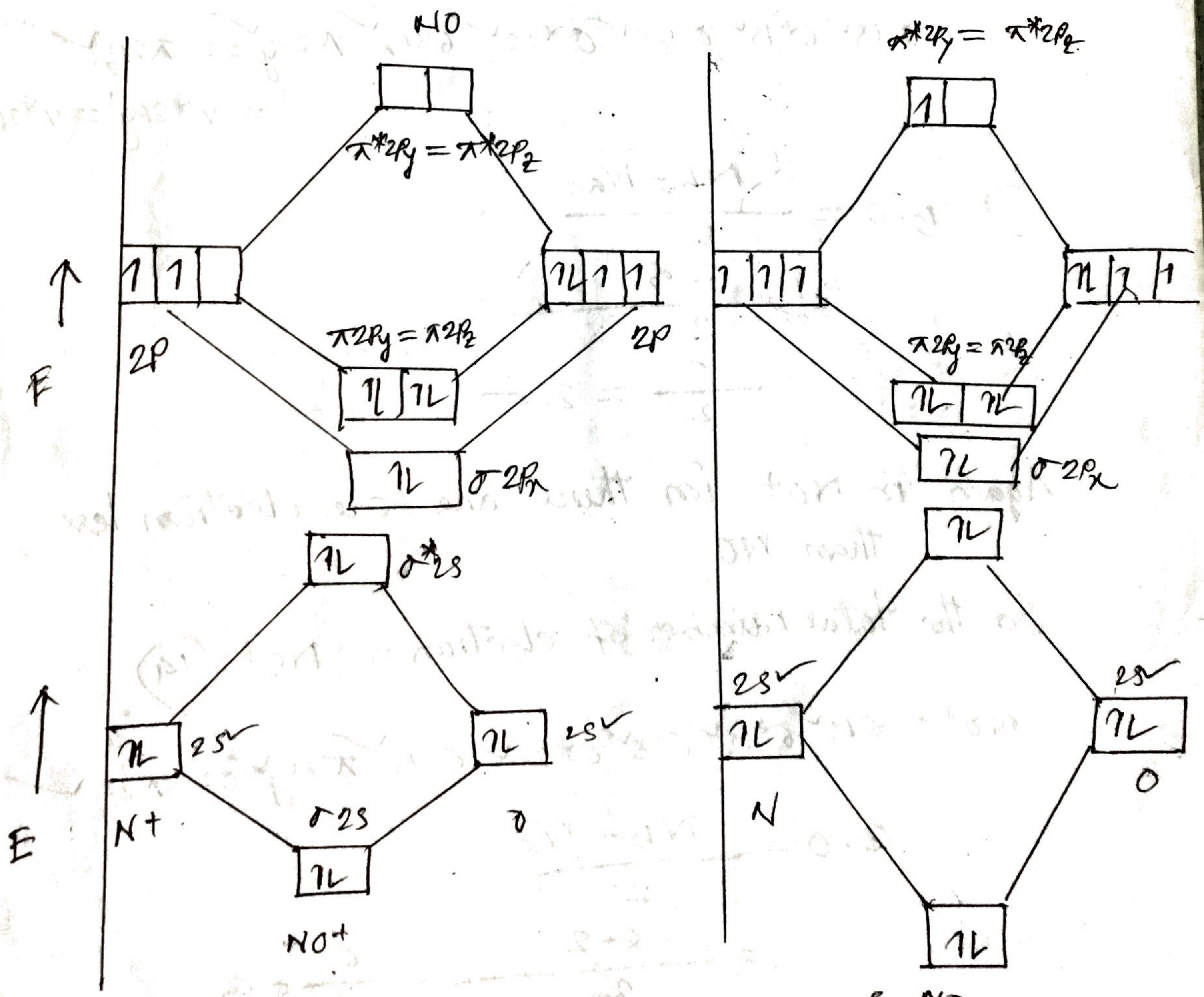
NO^+: $\sigma 1s^2\, \sigma^* 1s^2\, \sigma 2s^2\, \sigma^* 2s^2\, \sigma 2p_x^2\, \pi 2p_y^2 = \pi 2p_z^2$

$$B.O = \frac{N_b - N_a}{2}$$

$$= \frac{8-2}{2} = \frac{6}{2} = 3.$$

We know that, Bond order ∝ Bond Strength.
Hence the bond order of NO^+ is 3 and NO is 2.5
So the strength of NO^+ is greater than that of NO

or,
increasing the bond-order decrease the bond length. So the bond length of NO^+ is less than that of NO.



MO of NO

Q. N_2^+ ion less relaxable than N_2 But O_2^+ ion more relaxable than O_2 ? Explain this ——

Soln. Electronic configuration of N —

$N(7) \longrightarrow 1s^2 2s^2 2p^3$

Number of total electron in N_2 molecule $(7+7) = 14$

N_2 : $KK\ \sigma 2s^2\ \sigma^* 2s^2\ \sigma 2p_x^2\ \pi 2p_y^2 = \pi 2p_z^2$

$$B.O = \frac{N_b - N_a}{2}$$

$$= \frac{8-2}{2} = \frac{6}{2} = 3$$

In N_2^+ ion there are one electron less than N_2 so the total electron in N_2^+ is (13)

N_2^+ : $KK\ \sigma 2s^2\ \sigma^* 2s^2\ \sigma 2p_x^2\ \pi 2p_y^1 = \pi 2p_z^1$

$$B.O = \frac{N_b - N_a}{2}$$

$$= \frac{7-2}{2} = 5/2 = 2.5$$

We know that, Bond order $\propto$ Bond stability

So greater the Bond order increase the relaxation of the molecule

$B.O$ of $N_2 = 3$

$B.O$ of $N_2^+ = 2.5$

So the relaxation of N_2 is more than N_2^+ ——

Again,

Electronic Configuration of O atom

$O(8) \longrightarrow 1s^2 2s^2 2p_x^2 2p_y^1 2p_z^1$

Total electron of O_2 is $(8+8) = 16$

$$O_2 : KK\,\sigma 2s^2\,\sigma^* 2s^2\,\sigma 2p_x^2\,\pi 2p_y^2 = \pi 2p_z^2\,\pi^* 2p_y^1 = 2p_z^1$$

$$B.O = \frac{N_b - N_a}{2}$$

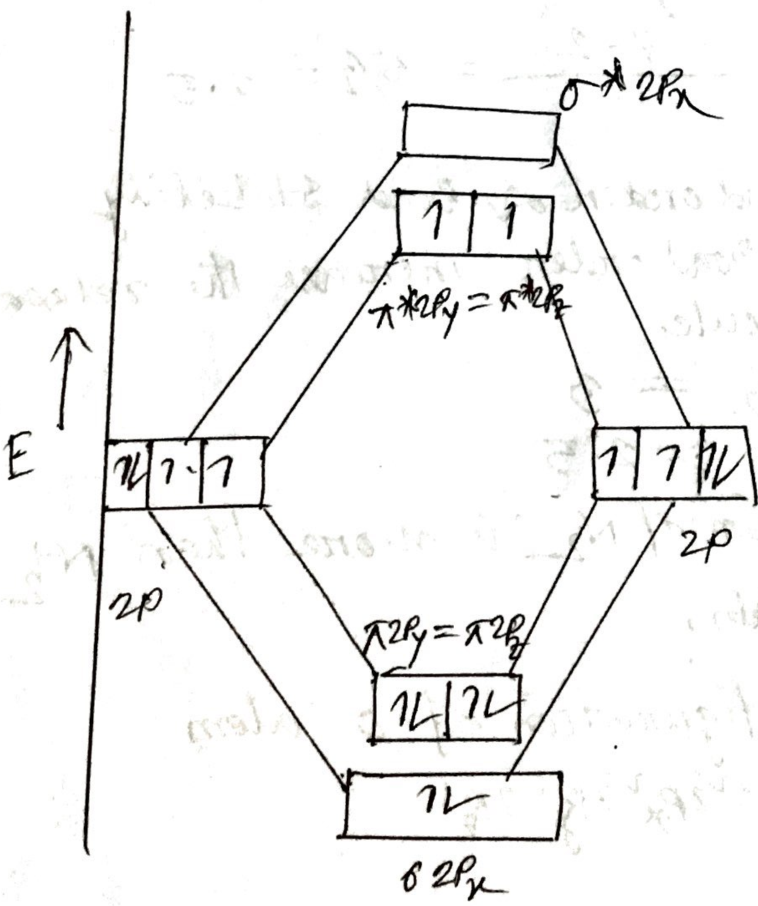
$$= \frac{8-4}{2} = \frac{4}{2} = 2$$

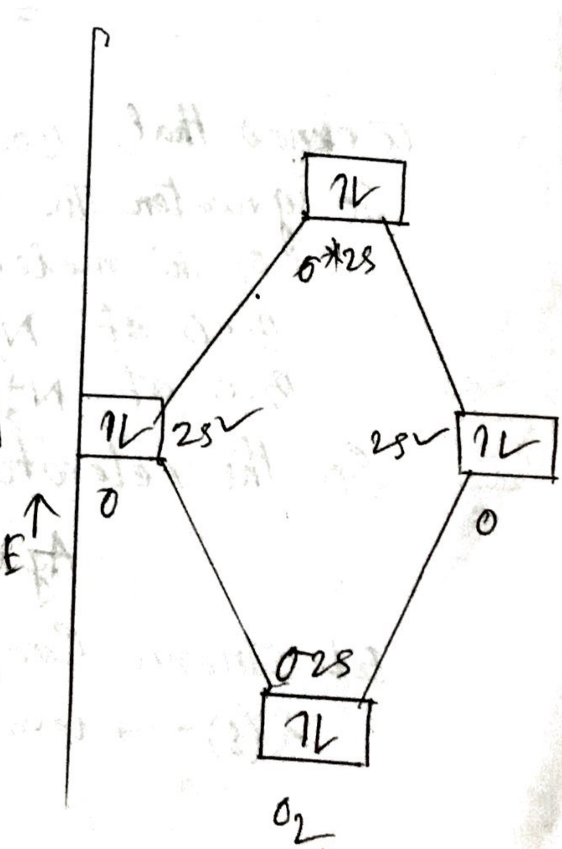
Again, in O_2^+ ion one electron less than O_2
So,

$$O_2^+ : KK\,\sigma 2s^2\,\sigma^* 2s^2\,\sigma 2p_x^2\,\pi 2p_y^2 = \pi 2p_z^2\,\pi^* 2p^1$$

$$B.O = \frac{8-3}{2} = 2.5$$

therefore, B.O of O_2 is 2 and B.O of O_2^+ is 2.5. So O_2^+ ion more relaxable than O_2





Q. Discuss the relaxation of the following molecules in (MOT) orbitals theory ?

Soln. O_2^+ ion: there are 15 electron in this molecules

O_2^+ : $KK\sigma 2s^2 \sigma^* 2s^2 \sigma 2p_x^2 \pi 2p_y^2 = \pi 2p_z^2 \pi^* 2p_y^1$

$$B.O = \frac{N_b - N_a}{2}$$

$$= \frac{8-3}{2} = 2.5$$

Again

O_2^- ion: Number of total electron (17). So the electronic configuration of O_2^-

O_2^- : $KK\sigma 2s^2 \sigma^* 2s^2 \sigma 2p_x^2 \pi 2p_y^2 = \pi 2p_z^2 \pi^* 2p_y^2 = \pi^* 2p_z^1$

$$B.O = \frac{N_b - N_a}{2}$$

$$= \frac{8-5}{2} = 1.5$$

Again O_2^{-2} ion: There are total Number of electron is 18.

So the electronic configuration of O_2^{2-} is

O_2^{2-} : $KK\sigma 2s^2 \sigma^* 2s^2 \sigma 2p_x^2 \pi 2p_y^2 = \pi 2p_z^2 \pi^* 2p_y^2 = \pi^* 2p_z^1 \sigma^* 2p_x^1$

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

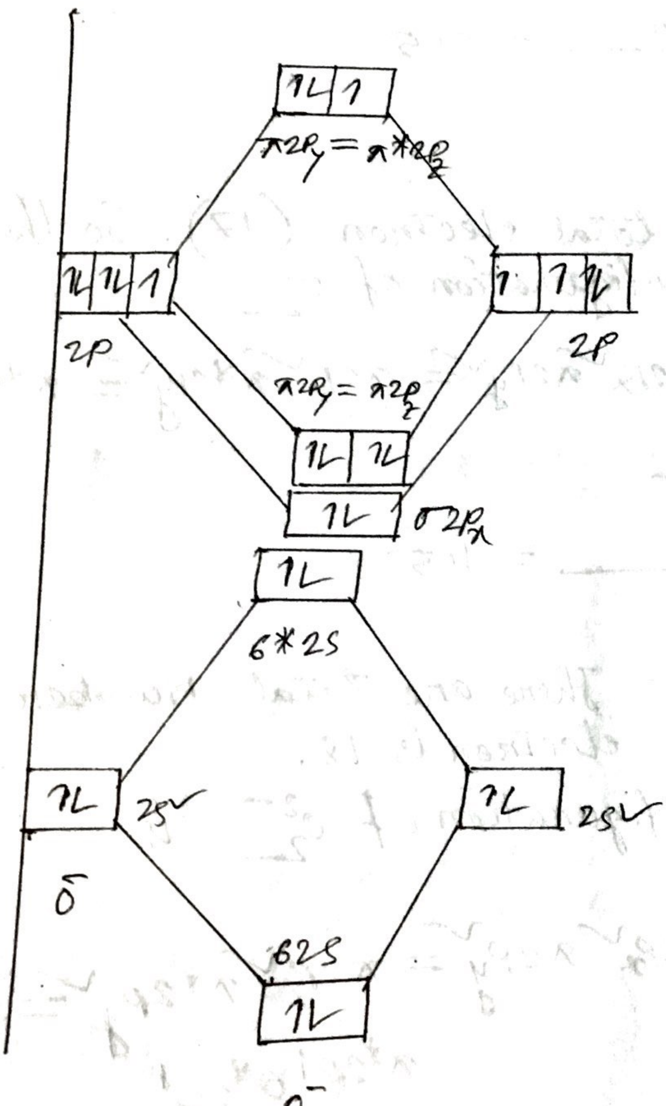
$$= \frac{8-6}{2}$$

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

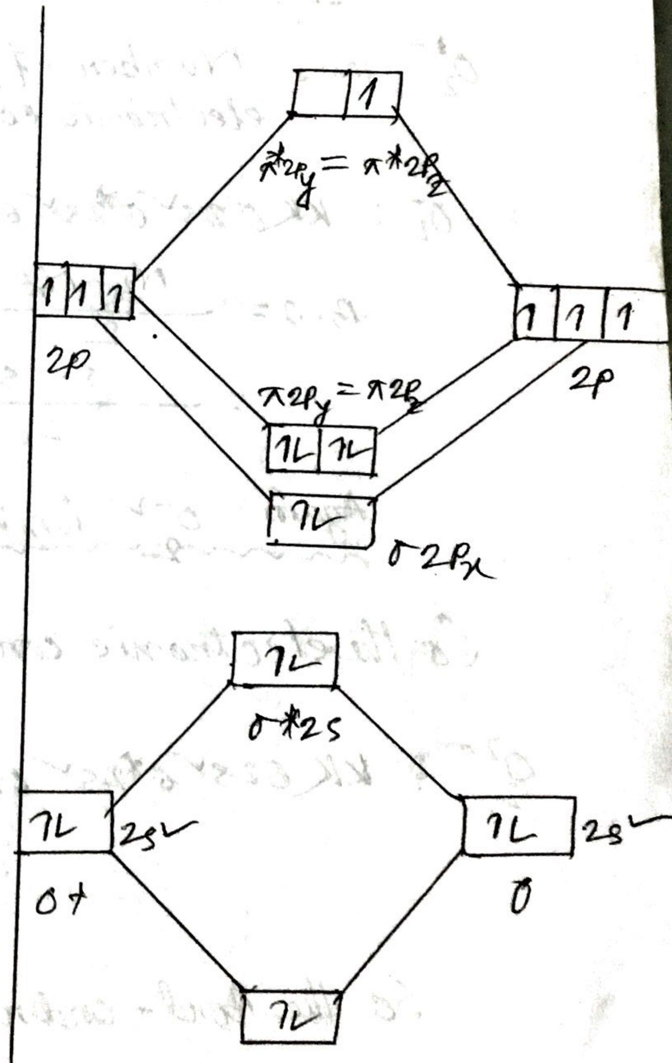
So the sequence of the molecule are

$O_2^+ > O_2^- > O_2^{-2}$

Therefore their relaxation are $O_2^+ > O_2^- > O_2^{-2}$



O_2^-



O_2^+

Q. Draw the figure of F_2 and calculate the Bond-order and prove that it is diamagnetic ?

Soln. Electronic configuration of F atom :

$F(9) \rightarrow 1s^2 2s^2 2p_x^2 2p_y^2 2p_z^1$

∴ So there are 18 electron in F_2 Molecule.

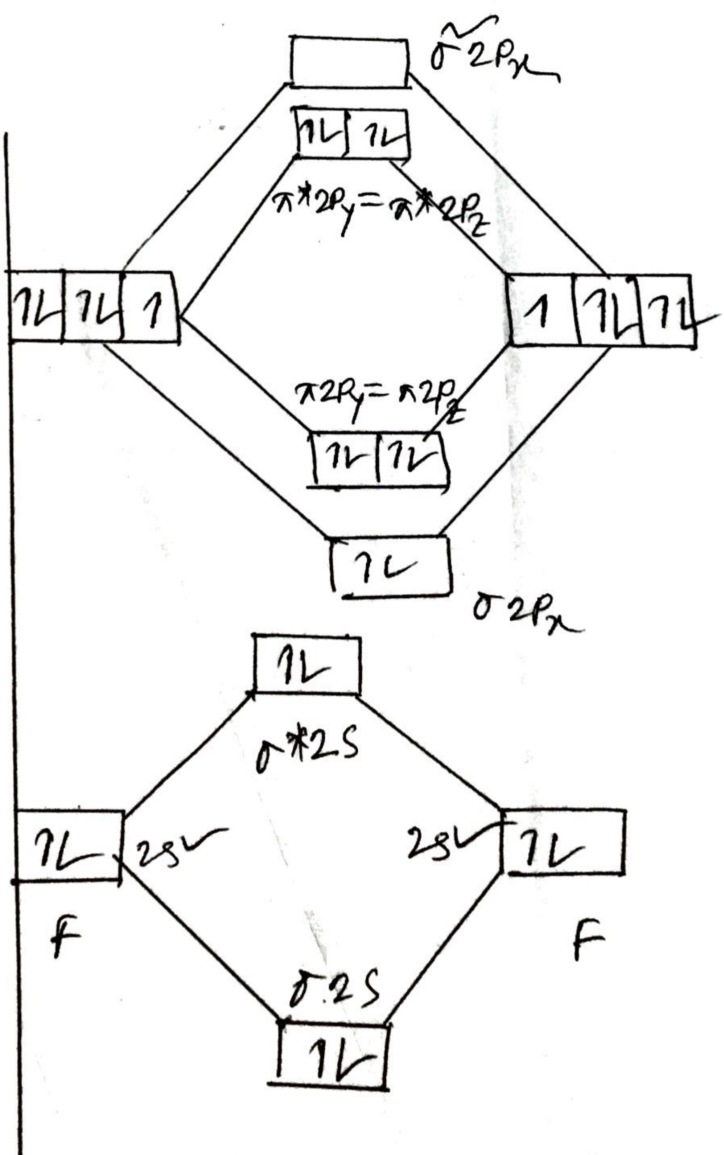
F_2 : $KK\ \sigma 2s^2\ \sigma^* 2s^2\ \sigma 2p_x^2\ \pi 2p^4\ \pi^* 2p^4$

$$B.O = \frac{N_b - N_a}{2}$$

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

$$= \frac{2}{2}$$

$$= 1$$



So F_2 molecule is diamagnetic in Nature