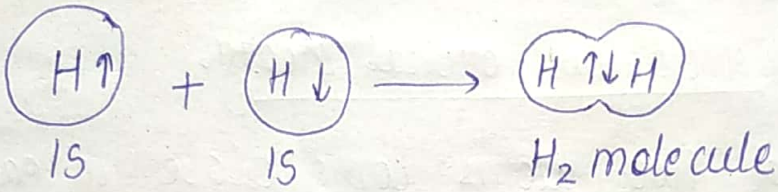
Valence Bond Theory

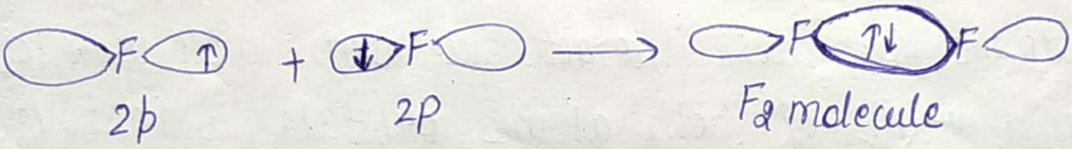
It was proposed by W. Heitler and F. London.

It explains the bonding of atomic orbitals.

The overlapping of atomic orbitals results in the formation of chemical bond and electrons are localized in the bond region due to overlapping.

Example →





Limitations of VBT

1. It fails to explain the stability of some molecule H_2^+, H_2^-
2. It does not explain the paramagnetic nature of O_2 molecule.
3. It fails to explain the bond strength of molecules eg O_2, O_2^+, O_2^-.

Molecular Orbital Theory (MOT)

Molecular Orbital theory was proposed by Hund and R.S. Mulliken. To explain the characteristics of molecules like their relative bond strength, paramagnetic and diamagnetic nature, this theory was developed. According to this theory, atomic orbitals combine and form a resultant orbital known as the molecular orbital in which the identity of both atomic orbitals is lost.

Main points of Molecular orbital theory:

1. When nuclei of two atoms come close to each other their atomic orbitals interact, to form molecular orbitals in which identity of both atomic orbitals is lost. (Figure 1)

e.g.

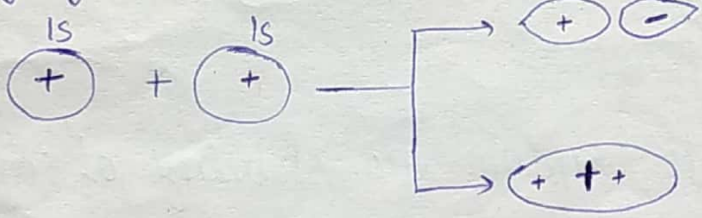


Figure ①

2. The number of molecular orbital formed is equal to the number of atomic orbitals involved in their formation. (Figure 1)

3. The electrons in the atomic orbitals are influenced by one nucleus, the electrons in the molecular orbitals are influenced by all the nuclei. (Figure 1)

4. Electrons are filled in the molecular orbitals in the same way as they are filled in atomic orbitals following Aufbau principle, Hund's rule of maximum multiplicity and Pauli exclusion principle.

(a) Aufbau principle: Molecular orbitals are filled in order of increasing energies

(b) Pauli Exclusion principle: A molecular orbital can have maximum two electrons and must have opposite spin.

(c) Hund's rule of maximum multiplicity: pairing electrons in degenerate molecular orbitals does not take place until each of them has got one electron each.

5. When two atomic orbitals combine, form two new orbitals called bonding molecular orbital and antibonding molecular orbital. (Figure 2)

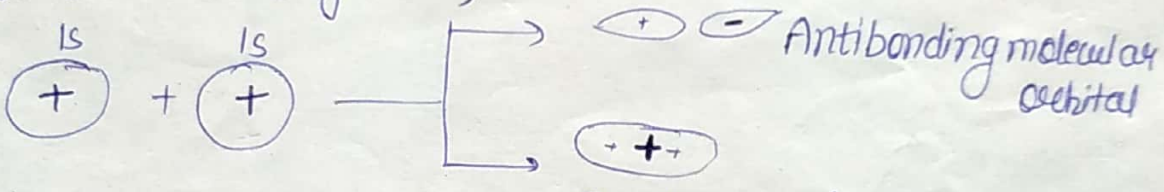


Fig (2)

6. The bonding molecular orbitals represented by σ, π, δ etc. whereas the corresponding antibonding molecular orbitals are represented by $\sigma^*, \pi^*, \delta^*$ etc.

Difference between Atomic and Molecular Orbital

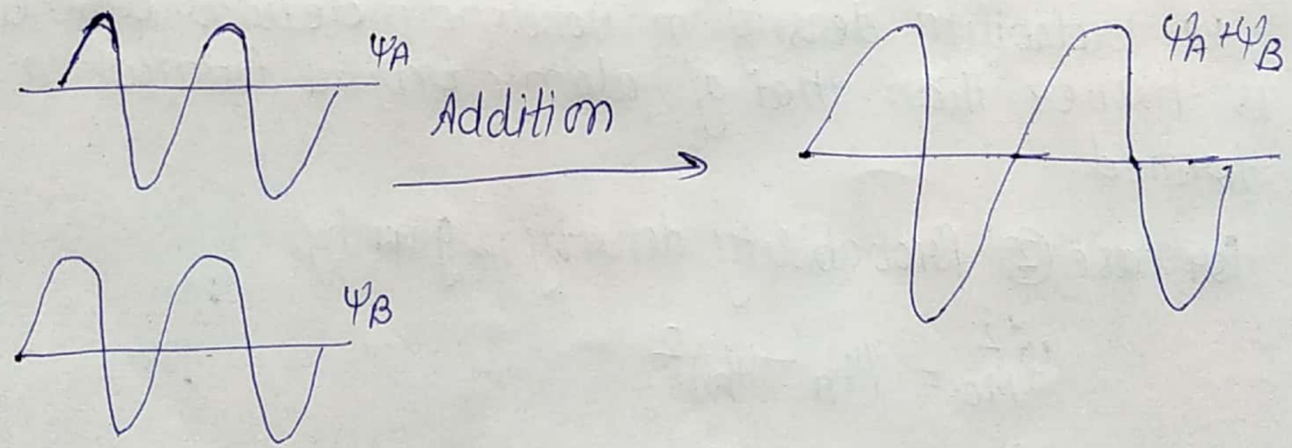
Atomic Orbital	Molecular Orbital
1. Their electron cloud extends around the nucleus of a single atom i.e. atomic orbital is mono centric.	1. Their electron cloud extends around the nuclei of bonded atoms in the molecule i.e. molecular orbital is polycentric.
2. They ~~are~~ have simple shapes	2. They have complex shapes.
3. They are represented by s, p, d, f etc.	3. They are represented by σ, σ^*, π, π^* etc.

Linear Combination of Atomic Orbitals (LCAO)

1. Formation of molecular orbitals explained on the basis of Linear combination of Atomic orbitals (LCAO)
2. Electrons considered as wave. Hence electron in atom is described by wave function ψ.
3. According to molecular orbital theory, electrons in molecule occupy molecular orbital.
4. Hence the wave function describing the molecular orbital obtained by method of Linear combination of atomic orbital
5. consider a molecule consist of two atoms A and B The atomic orbitals of these atoms represented by wave function ψ_A and ψ_B respectively.

There are two possible ways of linearly combining the atomic orbitals.

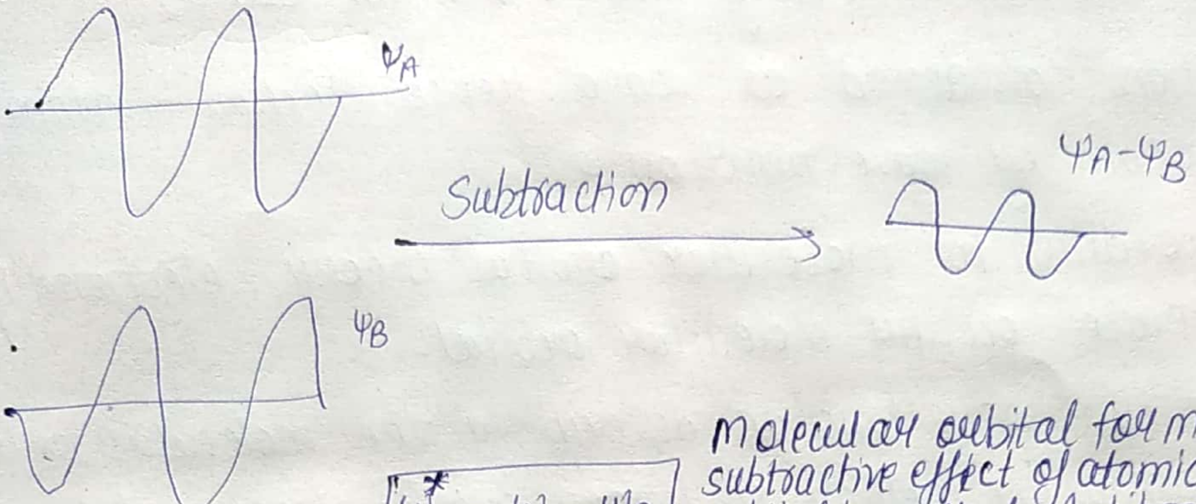
(i) Additive combination → where the sign of two wavefunction are same or when two waves are inphase



$$\psi_{MO} = \psi_A + \psi_B$$

The molecular orbital formed by additive effective of atomic orbitals is called Bonding molecular orbital.

(ii) Subtractive combination: where the signs of two wave functions are different or when two waves are out of phase:-



$\boxed{\psi^*_{MO} = \psi_A - \psi_B}$ molecular orbital formed by subtractive effect of atomic orbital is called Antibonding molecular orbital

~~(iii)~~ Probability density of ~~finding~~ electron is given by ψ^2

∴ for case ① Probability density is given by

$$\psi_{MO}^2 = (\psi_A + \psi_B)^2$$

$$\psi_{MO}^2 = \psi_A^2 + \psi_B^2 + 2\psi_A\psi_B$$

Hence $\psi_{MO}^2 > \psi_A^2 + \psi_B^2$

ie Probability density in Bonding molecular orbital is higher than that of atomic orbital from which it is formed.

for case ② Probability density is given by

$$\psi^{*2}_{MO} = (\psi_A - \psi_B)^2$$

$$\psi^{*2}_{MO} = \psi_A^2 + \psi_B^2 - 2\psi_A\psi_B$$

Hence $\psi^{*2}_{MO} < \psi_A^2 + \psi_B^2$

1. Probability density in Antibonding molecular orbital is lower than that of atomic orbital from which it is formed.

Hence Ⓐ Probability density is higher in Bonding molecular orbital means

→ electron density is located between nuclei of atoms

→ nuclei are shielded from each other and less repulsion between nuclei.

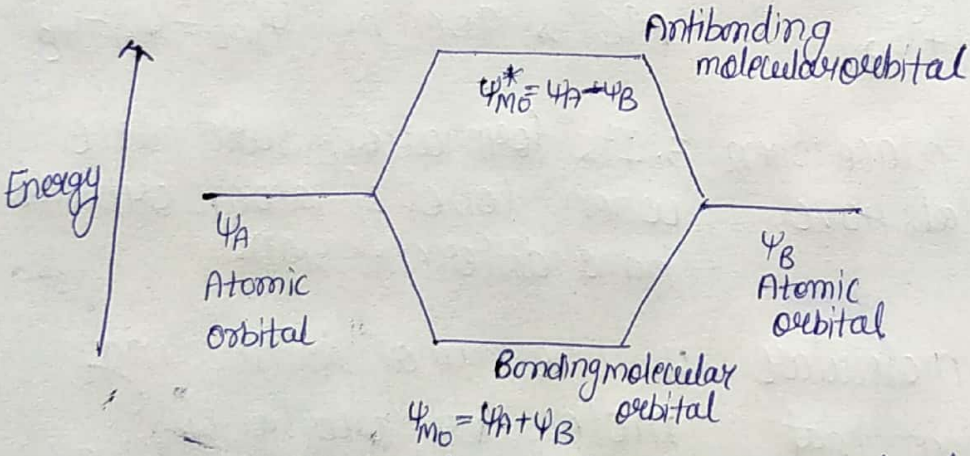
∴ energy of Bonding molecular orbital is lower than that of atomic orbitals.

Ⓑ Probability density is lower in Antibonding molecular orbitals

→ i.e. electron density is located away from nuclei

→ hence repulsion between nuclei is high.

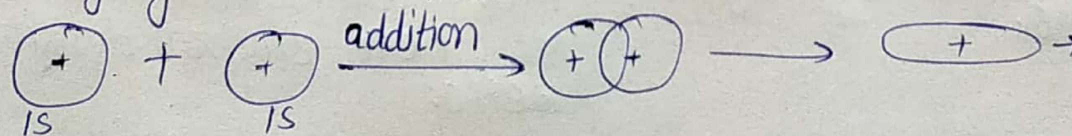
→ ∴ energy of Antibonding molecular orbital is higher than that of atomic orbitals.



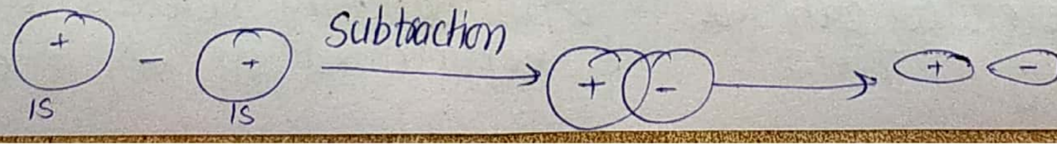
Energy level diagram or molecular orbital diagram.

for e.g 1s orbital of one hydrogen atom H_A combine with 1s orbital of other hydrogen atom H_B.

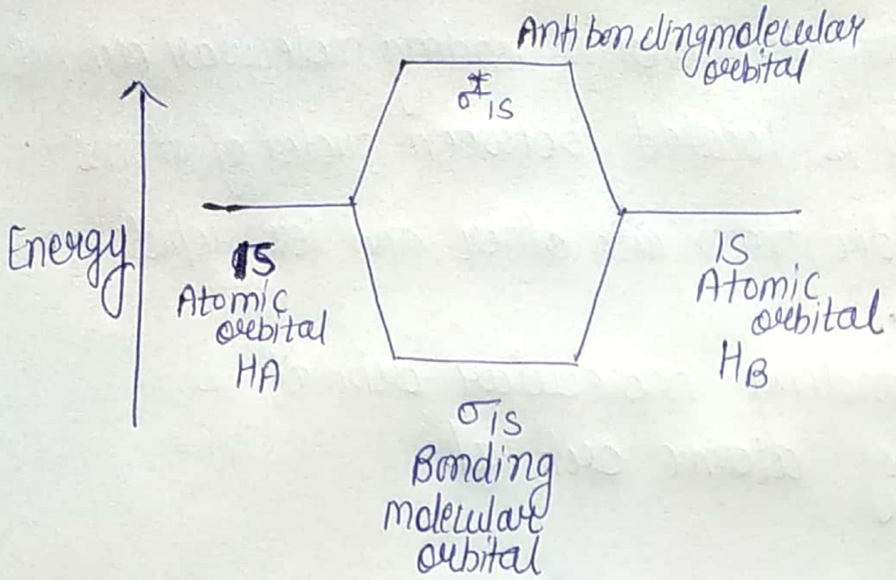
Two ways of combination.

①


σ_{1s} Bonding molecular orbital

②


σ^*_{1s} Antibonding molecular orbital



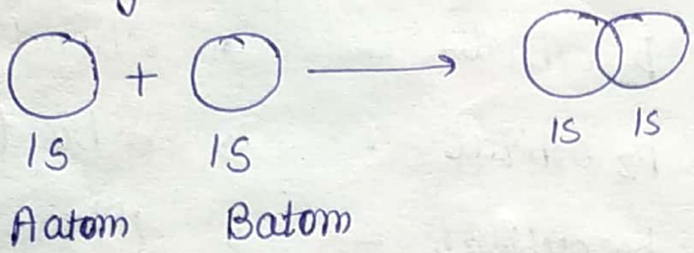
Difference between Bonding Molecular orbital and Antibonding molecular orbital

Bonding Molecular Orbital	Antibonding Molecular orbital
1. Molecular orbital formed by addition overlap of atomic orbitals are called Bonding molecular orbitals.	1. Molecular orbital formed by subtraction overlap of atomic orbitals are called Antibonding molecular orbitals.
2. Wave function of Bonding Mo is given by $\psi_{Mo} = \psi_A + \psi_B$	2. Wave function of Antibonding MO is given by $\psi^*_{MO} = \psi_A - \psi_B$
3. Its formation take place when lobes of atomic orbitals have same sign.	3. Its formation take place when lobes of atomic orbitals have different sign.
4. Energy of Bonding molecular orbital is lower than that of atomic orbital from which it is formed.	4. Energy of Antibonding molecular orbital is higher than that of atomic orbital from which it is formed.
5. Electron Probability of finding electron is more incase of Bonding MO.	5. Probability of finding electron is less in case of Antibonding MO. There is node in Antibonding MO where electron density is zero.
6. Bonding molecular orbitals represented by σ, π etc.	6. Antibonding molecular orbitals represented by σ*, π* etc.

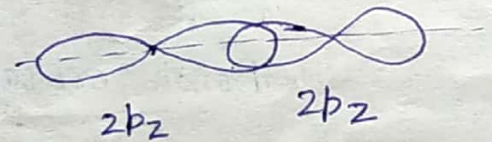
Condition for the combination of atomic orbitals

1. The atomic orbitals that are involved in the formation of molecular orbitals should have same energy.

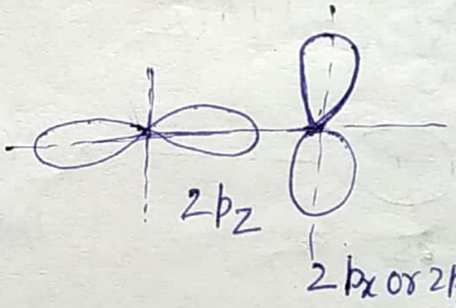
e.g 1s orbital ~~com~~ of one atom combine with 1s atomic orbital of another atom



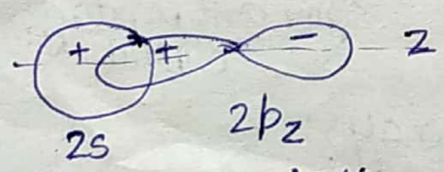
2. The combining atomic orbitals must have proper orientations or same symmetry with respect to molecular axis.



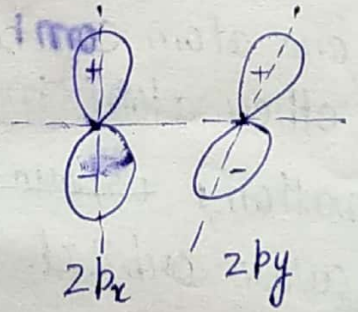
proper orientation (Same symmetry)



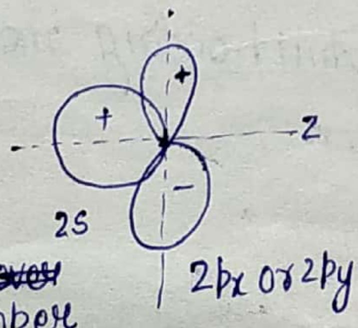
Improper orientation (no overlap)



proper orientation (same symmetry.)



Improper orientation (no overlap)



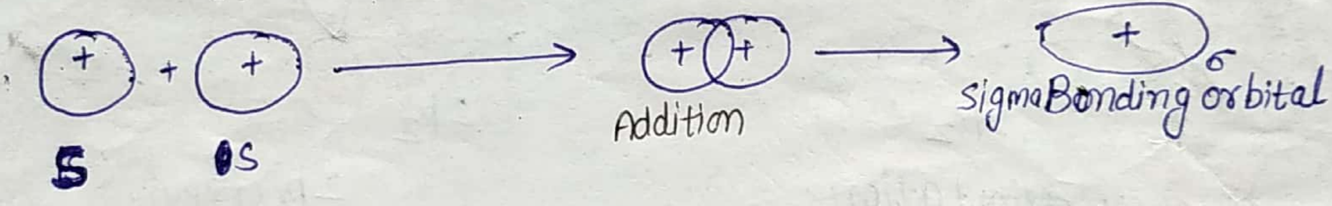
~~Over~~ Improper orientation (No overlap)

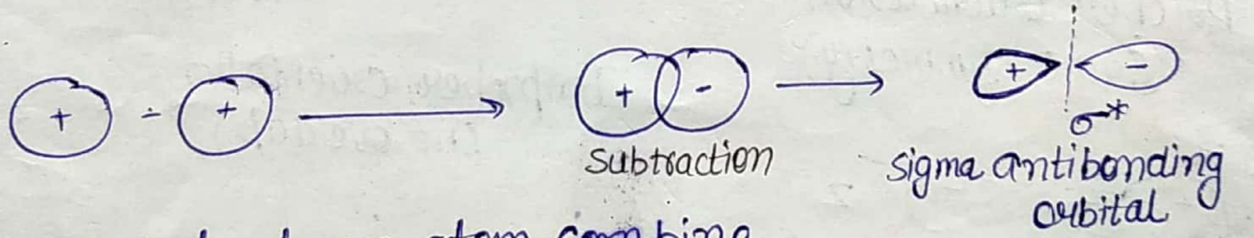
3. The extent of overlapping should be large. Greater the overlap, greater will be the electron density between nuclei.

Allowed combinations of Atomic Orbitals

1st orbital	2nd orbital	
s-orbital	s-orbital	→ σ bond
s orbital	p_z-orbital	→ σ bond
p_z orbital	p_z orbital	→ σ bond
p_y orbital	p_y orbital	→ π bond
p_x-orbital	p_x orbital	→ π bond

Combination of s-s orbitals





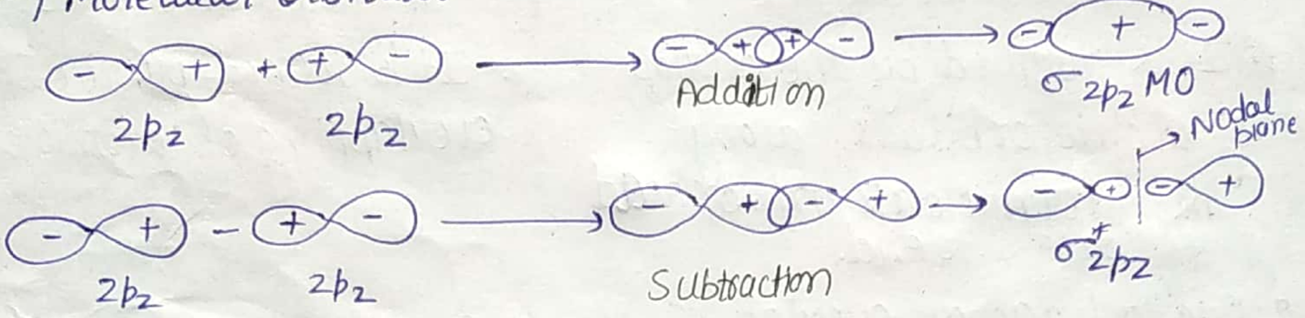
An s-orbital of one atom combine with s orbital of other atom in two ways:

(i) Additive combination ~~where signs of two~~ gives Bonding molecular orbital. (σ)

(ii) Subtractive combination gives Anti bonding molecular orbital (σ*).

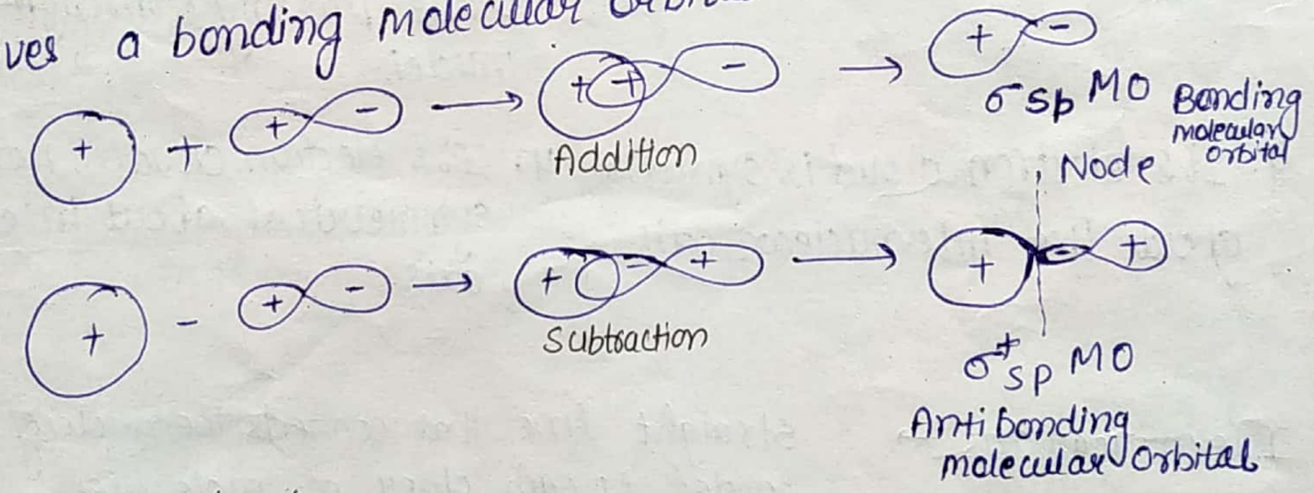
Combination of p_z-p_z orbitals

Overlap of two p orbitals, which have lobes pointing along the axis joining the nuclei resulting the formation of Bonding sigma molecular orbital (σ_{2p}) and antibonding sigma (σ^*) Molecular orbital.

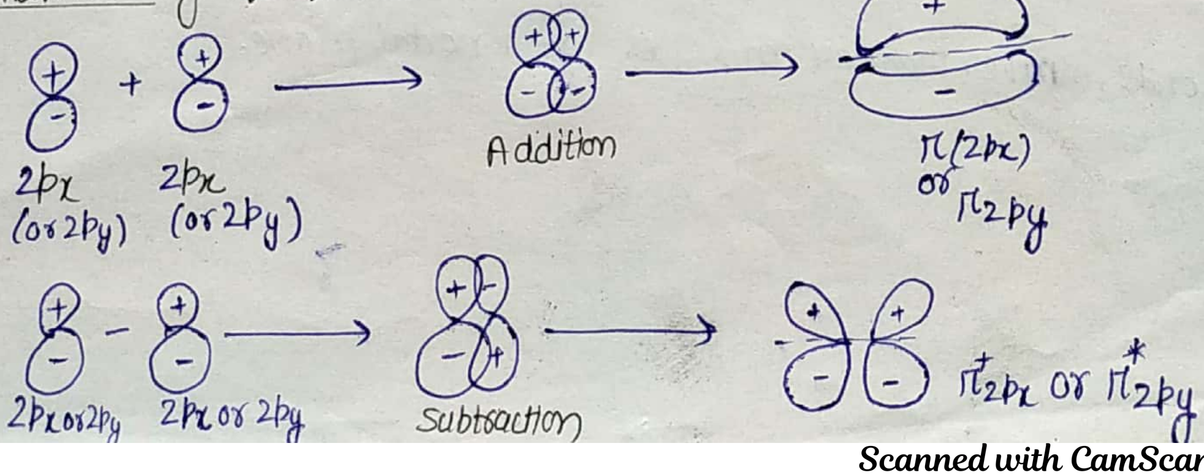


Combination of s-p orbitals

An s orbital combine with p orbital provided the lobes of p orbital are directed along the internuclear axis. When the overlapping lobes have same signs this gives a bonding molecular orbital.



Combination of p_x-p_x orbitals



for molecular orbitals

Difference between σ molecular orbital and π-molecular orbital

σ Molecular orbital	π-Molecular orbital
1. It is formed by the overlap of atomic orbitals along the internuclear axis or head to head or end to end.	1. It is formed by the sideways overlapping of atomic orbitals.
2. Due to head on overlap, the overlapping is maximum.	2. Due to sideway overlap, overlapping is less.
3. It consists of one electron cloud.	3. It consists of two electron clouds, one lying above and other lying below a plane passing through the nuclei.
4. Its electron cloud is symmetrical about the internuclear axis	4. Its electron cloud is not symmetrical about internuclear axis.

Internuclear axis → straight line that connects the nuclei of atoms bonded to each other in molecule.

In π bonds, internuclear axis lies in a nodal plane.

Energy Level Diagram for Molecular Orbitals

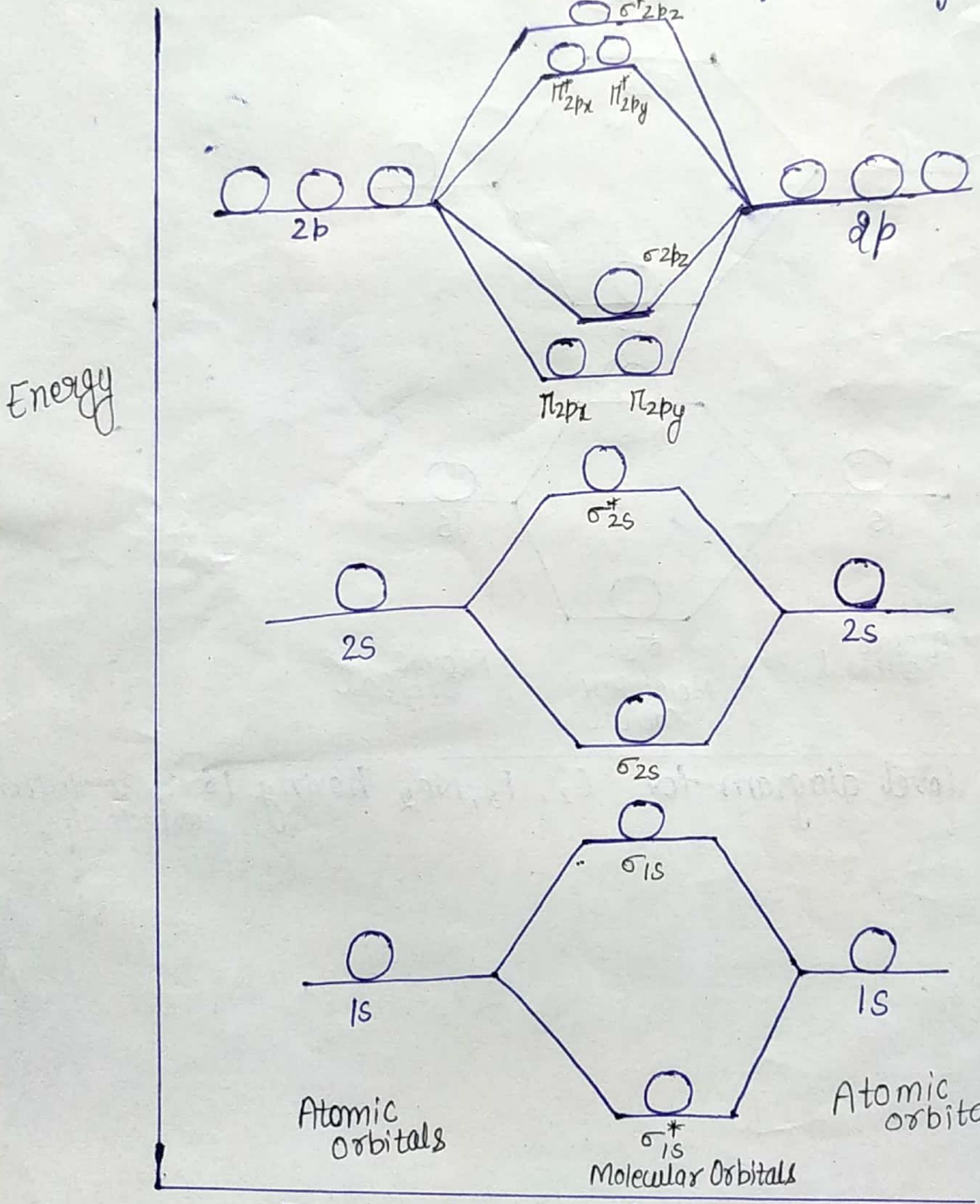
The relative energies of molecular orbitals in increasing order have been found to be as follows:

(a) For H_2 to N_2:

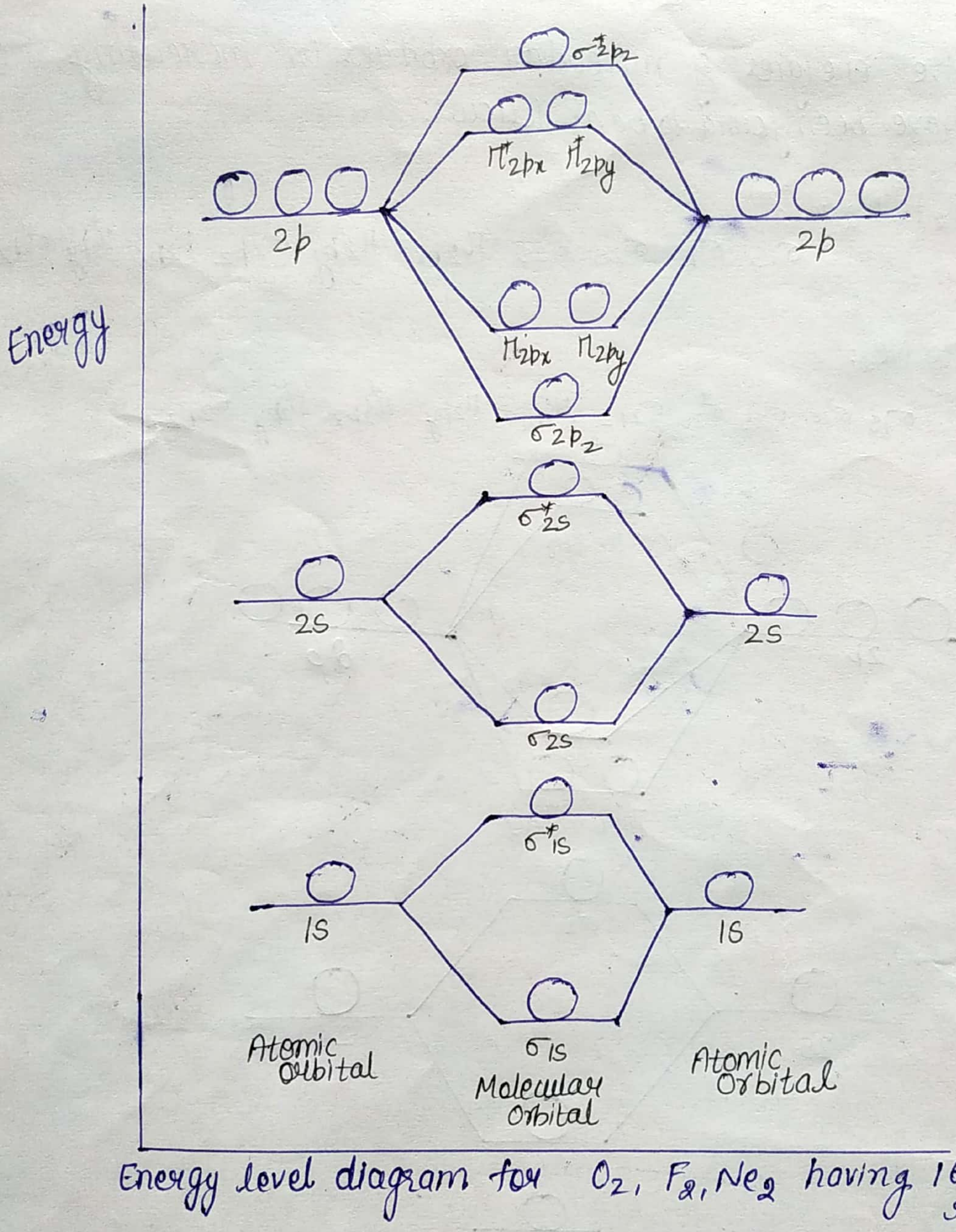
$$\sigma 1s \quad \sigma^* 1s \quad \sigma 2s \quad \sigma^* 2s \quad \pi 2p_x = \pi 2p_y \quad \sigma 2p_z \quad \pi^* 2p_x = \pi^* 2p_y \quad \sigma^* 2p_z$$

(b) For O_2 to Ne_2:

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



Energy level diagram for Li_2, B_2, C_2, N_2.



Energy level diagram for O_2, F_2, Ne_2 having 16, 18, 20 electron respectively.

Filling of Electrons in Molecular Orbitals

1. **Aufbau principle:** The orbital with lowest energy is to be filled first i.e. electrons enters various molecular orbital in the order of their increasing energies

For O_2, F_2, Ne_2

$$\sigma_{1s} < \sigma^*_{1s} < \sigma_{2s} < \sigma^*_{2s} < \sigma_{2p_z} < \pi_{2p_x} = \pi_{2p_y} < \pi^*_{2p_x} = \pi^*_{2p_y} < \sigma^*_{2p_z}$$

For B_2, C_2 N_2

$$\sigma_{1s} < \sigma^*_{1s} < \sigma_{2s} < \sigma^*_{2s} < \pi_{2p_x} = \pi_{2p_y} < \sigma_{2p_z} < \pi^*_{2p_x} = \pi^*_{2p_y} < \sigma^*_{2p_z}$$

2. **Pauli's Exclusion principle:** The maximum number of electrons in a molecular orbital is two and these should have opposite spins.

3. **Hund's Rule:** Pairing of electrons take place only when each molecular orbital of same energy has at least one electron each

~~$\sigma_{1s}^2 \; \sigma^{*2}_{2s} \; \sigma^2_{2s} \; \sigma^{*2}_{2s} \; \pi^1_{2p_x} = \pi^1_{2p_y}$~~

Bond Order of Molecule:

- Bond order determines the number of bonds in a molecule.
- It is defined as half of difference between the number of electrons present in bonding and antibonding molecular orbitals i.e.

$$\text{Bond order} = \frac{1}{2}\left(\text{No. of electrons in bonding molecular orbital} - \text{Number of electrons in antibonding molecular orbital}\right)$$

OR

$$B.O = \frac{1}{2}(N_b - N_a)$$

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Significance of Bond order

1) Bond order is a measure of strength of bond between two atoms.

2) Greater the value of bond order, greater is the stability of molecule.

3) Greater the bond order value is higher is the bond dissociation energy.

4) When the bond order is zero, Hence the molecule is unstable and it does not exist.

5) Bond order is inversely proportional to bond length.

$$\boxed{\text{Bond order} \propto \frac{1}{\text{Bond length}}} \quad \text{OR} \quad \boxed{B.O \propto \frac{1}{B.L}}$$

6) Bond order determines the number of bonds in a molecule.

Magnetic properties: Paramagnetic or Diamagnetic Nature of Molecules

a) Paramagnetic nature: A molecule is paramagnetic in nature, if it contains one or more unpaired electrons in the molecular orbitals.

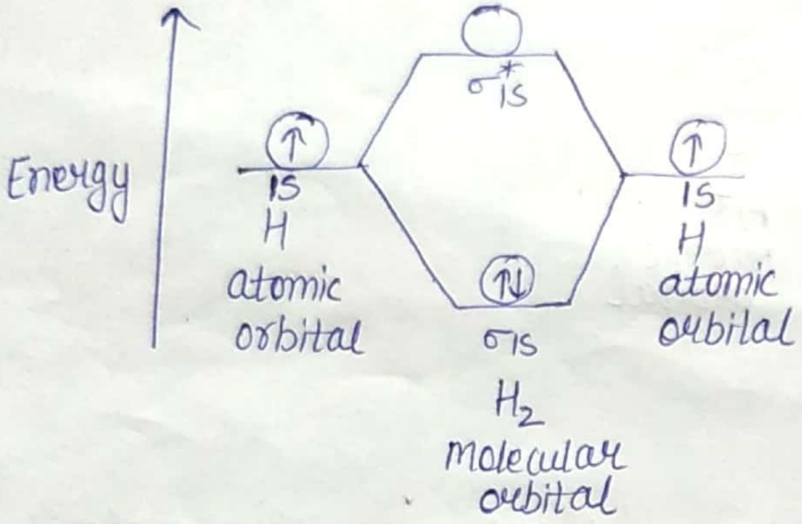
Greater ~~is~~ the number of unpaired electrons in molecular orbitals of substance, higher is paramagnetic character.

(b) Diamagnetic nature: If the molecule does not has any unpaired electron, then it will be diamagnetic in nature.

Homonuclear Diatomic molecules

① H_2 → Each hydrogen atom has 1 electron and hence. H_2 molecule has 2 electrons. & configuration of H atom is $1s^1$
Therefore, electronic configuration of H_2 is $\boxed{\sigma_{1s}^{2}}$
Molecular orbital

Energy level diagram of H_2



Bond order → $\frac{1}{2} \times$ (Number of electrons in Bonding molecular orbital − Number of electrons in Antibonding molecular orbital)

No. of electrons in Bonding Molecular orbital = 2

No. of electrons in Anti Bonding Molecular orbital = 0

Bond order = $\frac{1}{2} \times (2-0) = \frac{1}{2} \times 2 = 1$

Bond order of H_2 molecule = 1

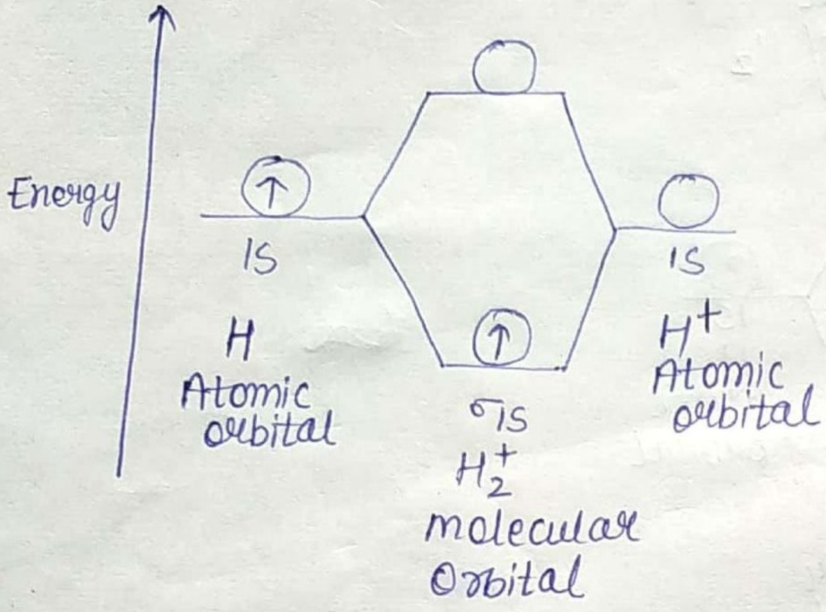
Magnetic properties → H_2 molecule ~~contains~~ / does not have any unpaired electron in molecular orbital.
Therefore it is diamagnetic in nature.

2. H_2^+ → H_2^+ has only one electron.

Molecular orbital Electronic configuration of H_2^+ is σ_{1s}^1

$H_2^+ \rightarrow \underset{1s^1}{H} + \underset{1s^0}{H^+}$ → configuration

Energy level diagram



Bond order = $\frac{1}{2}$ × (Number of electrons in Bonding Molecular orbital − Number of electrons in Antibonding molecular Orbital)

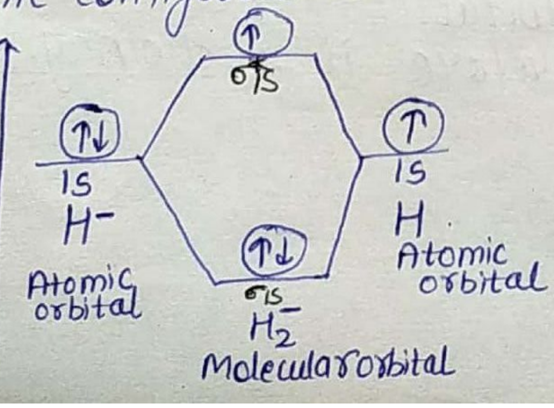
$= \frac{1}{2} \times (1-0) = \boxed{\frac{1}{2}}$ (No. of electrons in Bonding MO = 1, No. of electrons in Antibonding MO = 0)

Magnetic character → H_2^+ has one electron ∴ it is paramagnetic in nature.

3. H_2^- → It has 3 electrons

This is formed by combination of one hydrogen atom having one electron in 1s orbital with hydrogen ion having 2 electrons. H_2^- formed by combination of H^- and H orbitals.

Molecular orbital Electronic configuration is $\sigma_{1s}^2 \, \sigma_{1s}^{*1}$ and for H^- configuration is $1s^2$



Bond order $= \frac{1}{2}(N_b - N_a)$

$N_b = 2$ $N_a = 1$

$= \frac{1}{2} \times (2-1) = \boxed{\frac{1}{2}}$

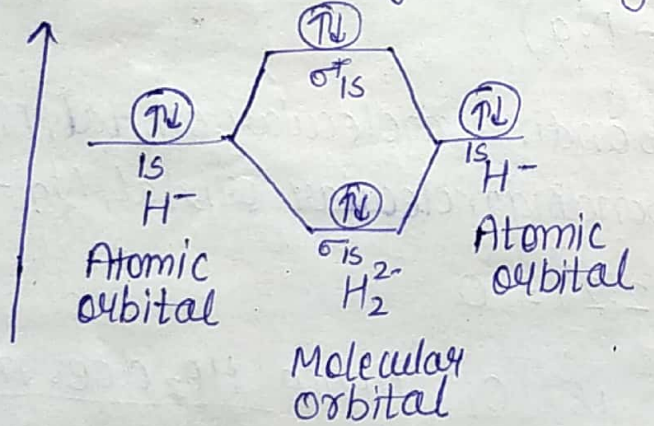
Magnetic character → It has one unpaired electron in σ^*_{1s} ∴ it is paramagnetic in nature

Molecule	Total electrons	Molecular orbital Electronic Configuration	Bond order	Magnetic Behaviour
H_2^+	1	σ_{1s}^1	$\frac{1}{2}$	Paramagnetic
H_2	2	σ_{1s}^2	1	Diamagnetic
H_2^-	3	$\sigma_{1s}^2\ \sigma_{1s}^{*1}$	$\frac{1}{2}$	Paramagnetic

④ ~~He_2~~ $H_2^{2+} \rightarrow H_2^{2+}$ has 0 electrons
∴ It does not exist

⑤ $H_2^{2-} \rightarrow H_2^{2-}$ has $2+2 = 4e^-$

Molecular orbital Electronic configuration of H_2^{2-} is $\sigma_{1s}^2\ \sigma_{1s}^{*2}$



Bondorder = $\frac{1}{2}(N_b - N_a)$

$N_b = 2$

$N_a = 2$

Bond order $= \frac{1}{2}(2-2)$

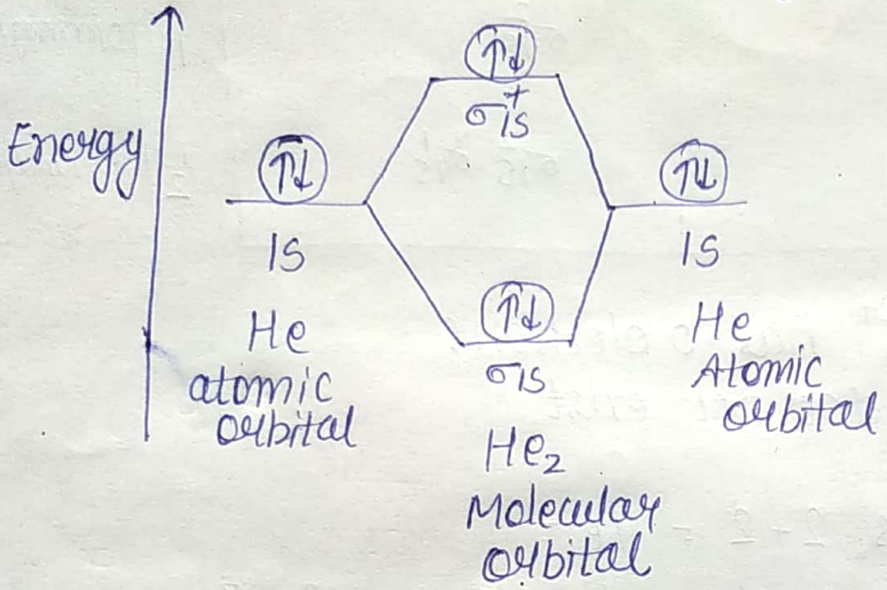
$= 0$

It means H_2^{2-} does not exist it has 0 bond order
H_2^{2-} is not stable molecule.

⑥ He_2 → He_2 is formed by combination of two He atoms having 2 electrons each. Its configuration is $1s^2$

∴ It has 4 electrons

Molecular Orbital electronic configuration is $\boxed{\sigma_{1s}^2 \overset{*}{\sigma}_{1s}^2}$



Bond order = $\frac{1}{2} \times (N_b - N_a)$

No. of electrons in Bonding molecular orbital, $N_b = 2$

No. of electrons in Antibonding molecular orbital, $N_a = 2$

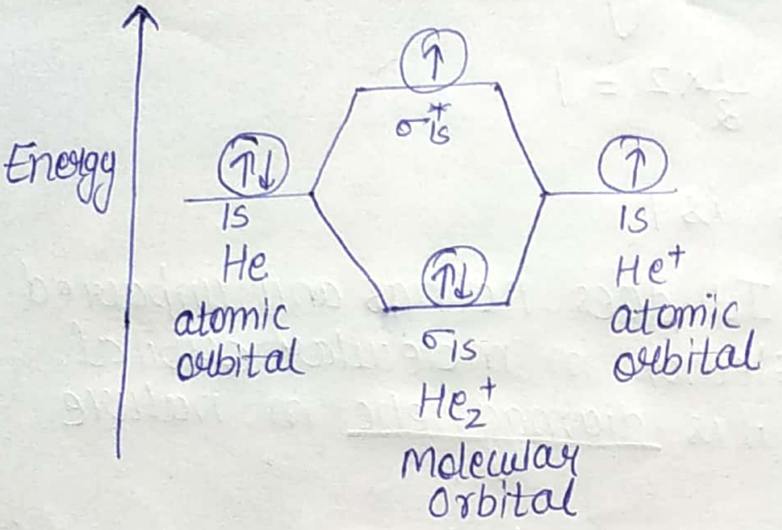
Bond order = $\frac{1}{2} \times (2-2) = 0$

Bond order of He_2 is $\boxed{0}$, Hence He_2 does not exist.

⑦ He_2^+ → It is formed from He atom and He^+ ion.
configuration of He is $1s^2$ and configuration of He^+ is $1s^1$

He_2^+ has 3 electrons.

Molecular orbital electronic configuration is $\boxed{\sigma_{1s}^2 \sigma_{1s}^{*1}}$.



Bond order $= \frac{1}{2} \times (N_b - N_a)$

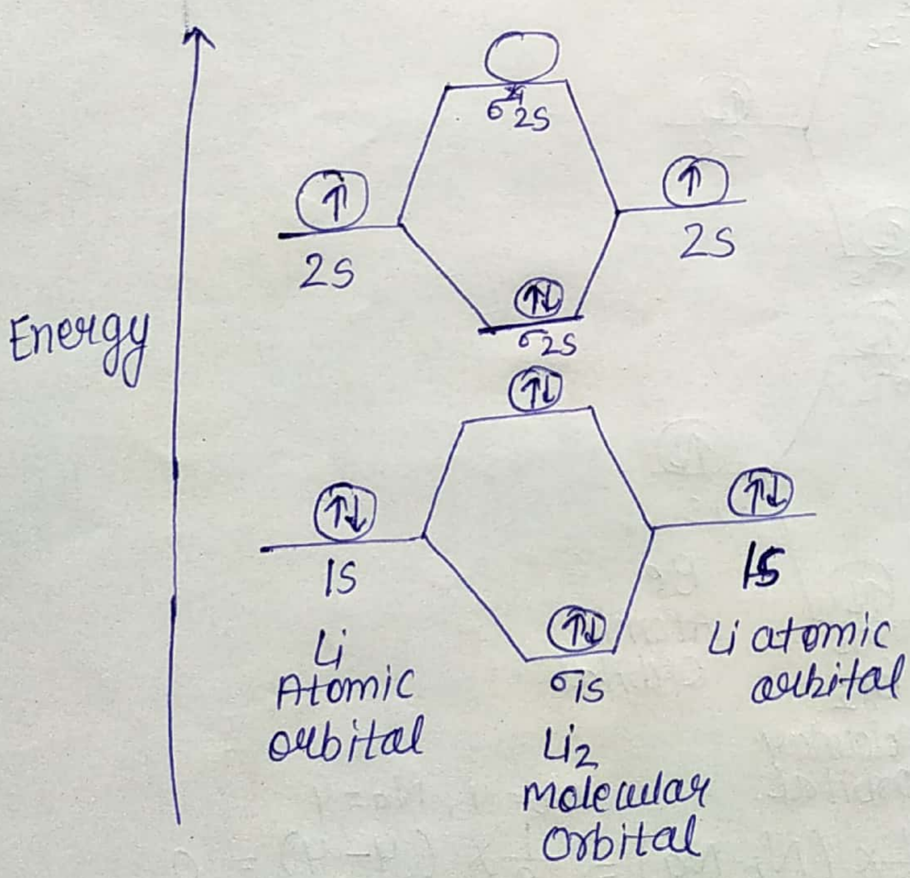
$N_b = 2$, $N_a = 1$

Bond order $= \frac{1}{2} \times (2-1)$
$= \frac{1}{2}$

He_2^+ can exist, but it is not very stable.

⑧ Li_2 → Li has 3 electrons and configuration of Li is $1s^2 2s^1$ ∴ Li_2 will have 6 electrons.

∴ Molecular orbital electronic configuration is $\sigma_{1s}^2 \sigma_{1s}^{*2} \sigma_{2s}^2$



B.O = Bond order → $\frac{1}{2} \times (N_b - N_a)$

No. of electrons in Bonding molecular orbital, $N_b = 4$

No. of electrons in Antibonding molecular orbital, $N_a = 2$

$B.O = \frac{1}{2} \times (4-2) = \frac{1}{2} \times 2 = 1$

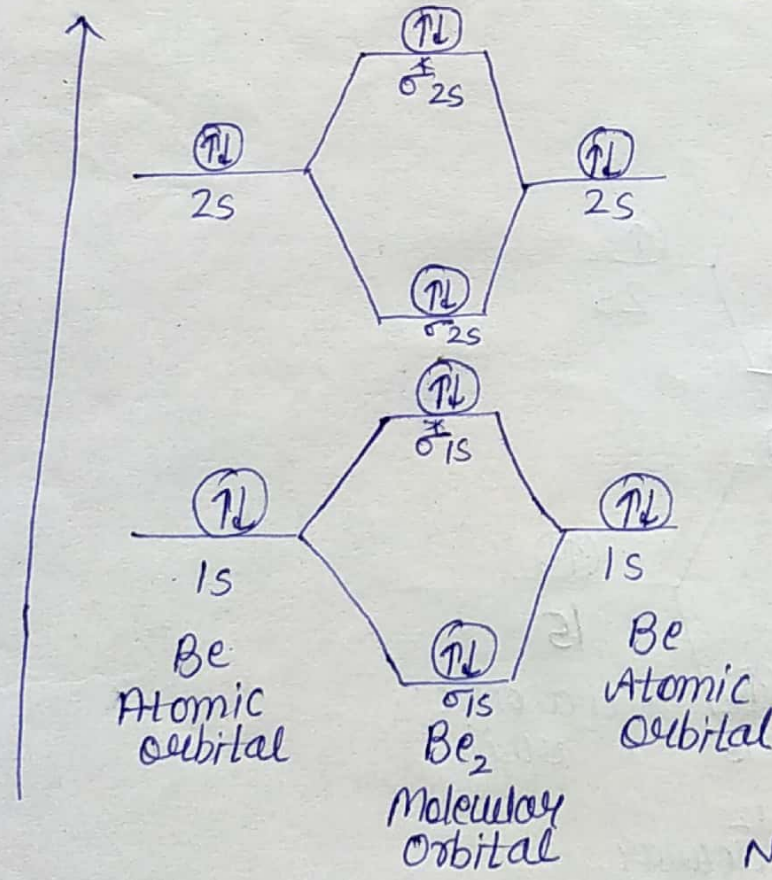
Bond order of Li_2 is 1

Magnetic behaviour → It does not has any unpaired electron in molecular orbital.
∴ it is diamagnetic in nature

⑨ Be_2 → Beryllium has four electrons and its configuration is $1s^2 2s^2$

Hence Be_2 Molecule has 8 electrons.

Molecular orbital electronic configuration is $\sigma_{1s}^2 \overset{*}{\sigma}_{1s}^2 \sigma_{2s}^2 \overset{*}{\sigma}_{2s}^2$



$N_b = 4, \ N_a = 4$

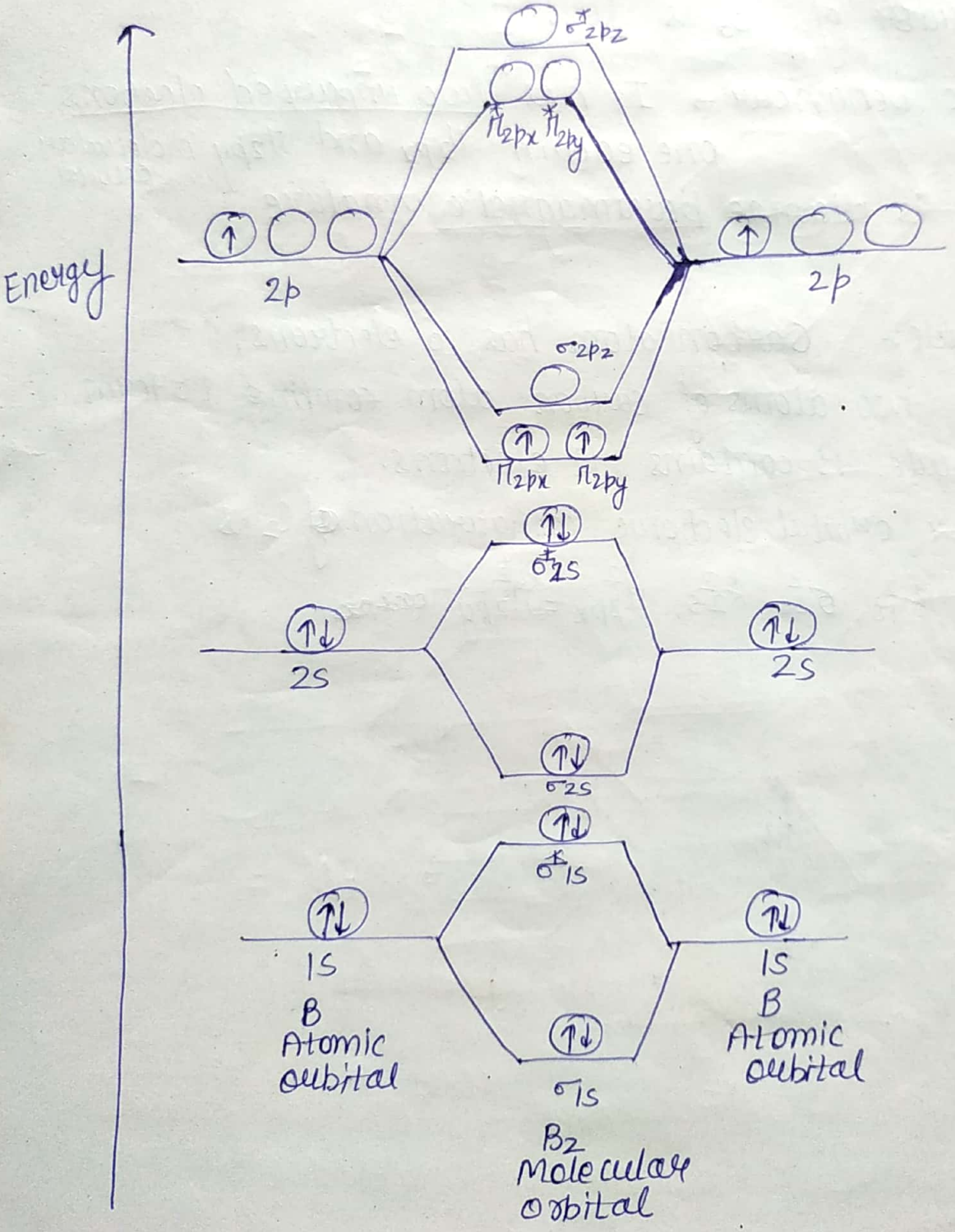
$\text{Bond order} = \frac{1}{2} \times (N_b - N_a) = \frac{1}{2} \times (4-4) = 0$

Bond order of Be_2 is 0 Hence this molecule does not exist.

⑩ B_2 → Boron atom has 5 electrons and its configuration is $1s^2 2s^2 2p^1$
Hence B_2 molecule has 10 electrons.

When two atoms of Boron combine to form B_2 molecule, ∴ it contains 10 electrons.

Molecular orbital electronic configuration of B_2 is $\boxed{\sigma_{1s}^2 \overset{*}{\sigma}{}_{1s}^2 \sigma_{2s}^2 \overset{*}{\sigma}{}_{2s}^2 \pi_{2p_x}^1 = \pi_{2p_y}^1}$



Bond order $= \frac{1}{2} \times (N_b - N_a)$

No. of electrons in Bonding molecular orbital, $N_b = 6$

No. of electrons in Antibonding molecular orbital, $N_a = 4$

$B.O = \frac{1}{2} \times (6-4) = \frac{1}{2} \times 2 = 1$

Bond order of B_2 is $\boxed{1}$.

Magnetic behaviour → It has <u>two unpaired electrons</u> one each in π_{2p_x} and π_{2p_y} molecular orbital

∴ It is ~~diamag~~ <u>paramagnetic</u> in nature

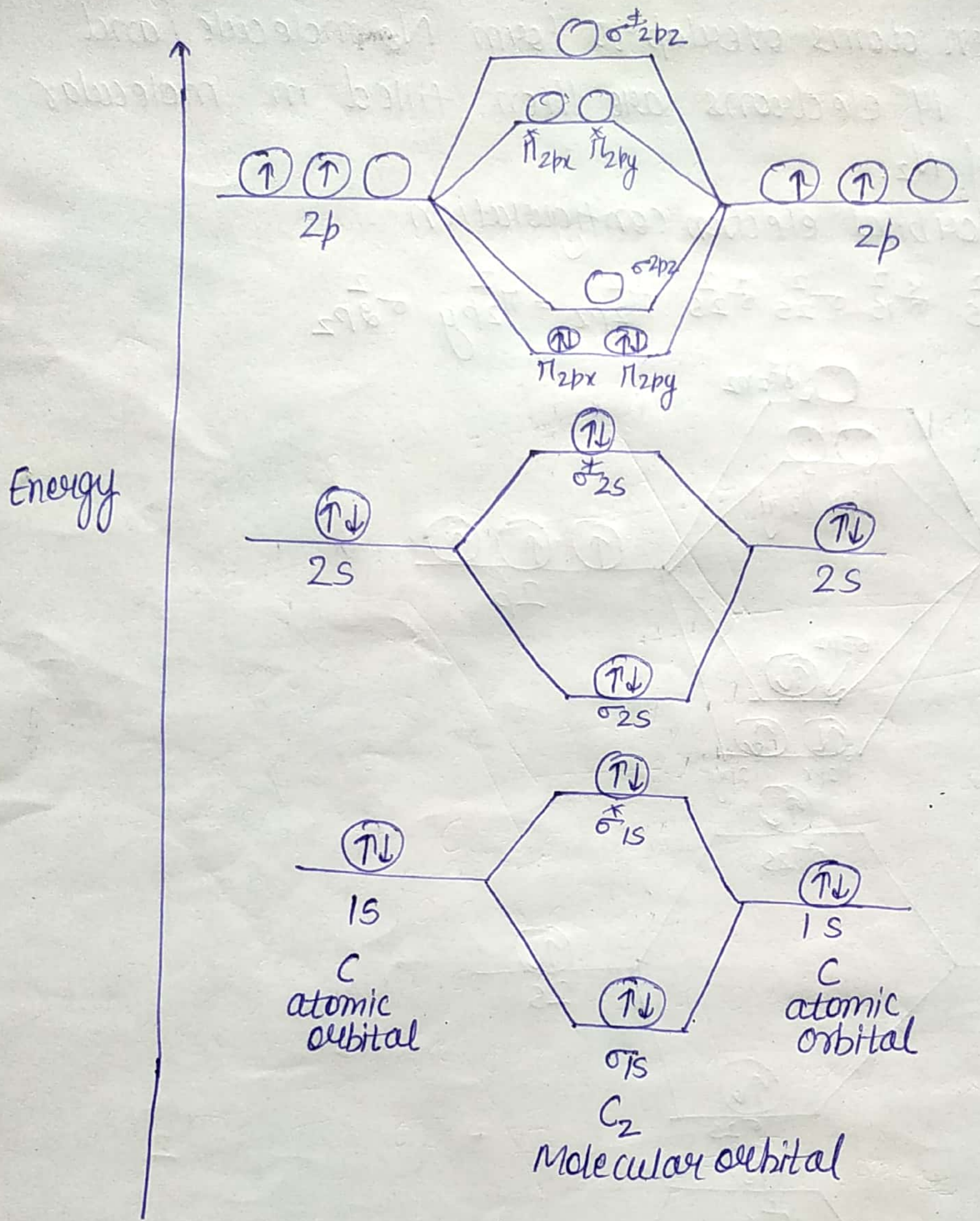
⑮ C_2 Molecule:- Carbon atom has 6 electrons & its configuration is $1s^2 2s^2 2p^2$

When two atoms of carbon atom combine to form C_2 molecule, it contains 12 electrons.

Molecular orbital electronic configuration of C_2 is

$\sigma^2_{1s}, \overset{*}{\sigma}{}^2_{1s}, \sigma^2_{2s}, \overset{*}{\sigma}{}^2_{2s}, \pi^2_{2p_x} = \pi^2_{2p_y}$ ~~σ_{2p_z}~~

Energy level diagram for C_2



Bond order = $\frac{1}{2} \times (N_b - N_a)$, $N_b = 8$, $N_a = 4$

$B.O = \frac{1}{2} \times (8-4) = \frac{1}{2} \times 4 = 2$

∴ C_2 is a stable molecule.

Magnetic behaviour :- All the (~~molecules~~) electrons are paired in molecular orbital.

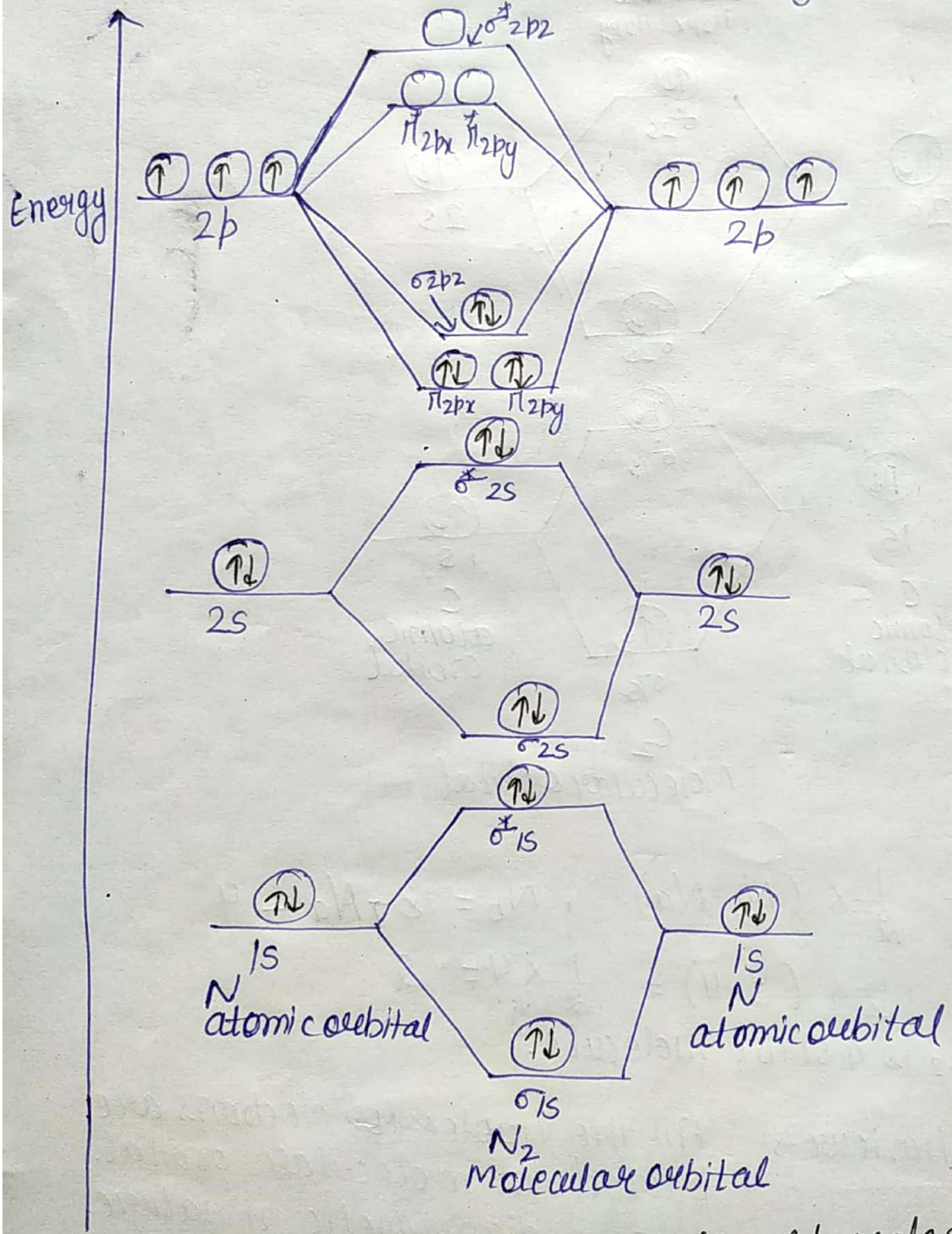
∴ It is diamagnetic in nature.

⑪ N_2 molecule → Nitrogen has 7 electrons, it has configuration $\boxed{1s^2 2s^2 2p^3}$.

Two nitrogen atoms overlap to form N_2 molecule and total of 14 electrons are then filled in molecular orbital of N_2.

Molecular orbital electron configuration

$$\sigma_{1s}^2 \; \overset{*}{\sigma}{}_{1s}^2 \; \sigma_{2s}^2 \; \overset{*}{\sigma}{}_{2s}^2 \; \pi_{2p_x}^2 = \pi_{2p_y}^2 \; \sigma_{2p_z}^2$$



Energy level diagram for N_2 molecule

Bond order : $\frac{1}{2} \times (N_b - N_a)$

$N_b = 10$
$N_a = 4$

Bond order $= \frac{1}{2} \times (10-4) = \frac{6}{2} = 3$

Bond order for $N_2 = \boxed{3} \rightarrow \boxed{N \equiv N}$
It is stable molecule

Magnetic behaviour : N_2 has no any unpaired electrons in molecular orbital
OR
It has paired electrons in molecular orbital

$\therefore$ N_2 is diamagnetic in nature.

Q. Write the electronic configuration of N_2, N_2^+, N_2^- and N_2^{2-}. Establish their stability order based on calculation of bond order. Also write their magnetic character.

~~Note~~ ① Electronic configuration of $\underset{(14e^-)}{N_2}$ is $\sigma_{1s}^2 \overset{*}{\sigma}{}_{1s}^2 \sigma_{2s}^2 \overset{*}{\sigma}{}_{2s}^2 \pi_{2p_x}^2 = \pi_{2p_y}^2 \sigma_{2p_z}^2$

~~N~~ →

Bondorder $= \frac{1}{2} \times (N_b - N_a)$, $N_b = 10$, $N_a = 4$

$= \frac{1}{2} \times (10-4) = \frac{6}{2} = 3$

B.O of $N_2 = 3$

Magnetic character = All electrons are paired in molecular orbital
$\therefore$ it is diamagnetic in nature

② Electronic configuration of $\underset{(13e^-)}{N_2^+}$ is $\sigma_{1s}^2 \overset{*}{\sigma}_{1s}^2 \sigma_{2s}^2 \overset{*}{\sigma}_{2s}^2 \pi_{2p_x}^2 = \pi_{2p_y}^2 \sigma_{2p_z}^1$

$B.O = \frac{1}{2} \times (N_b - N_a)$, $N_b = 9$ $N_a = 4$

$B.O = \frac{1}{2}(9-4) = \frac{5}{2} = 2.5$

Bond order for N_2^+ is $\boxed{2.5}$

Magnetic character :- It has one unpaired electron in σ_{2p_z} molecular orbital

∴ N_2^+ is $\boxed{\text{para magnetic}}$ in nature.

③ Electronic configuration of $\underset{(15e^-)}{N_2^-}$ is $\sigma_{1s}^2 \overset{*}{\sigma}_{1s}^2 \sigma_{2s}^2 \overset{*}{\sigma}_{2s}^2 \pi_{2p_x}^2 = \pi_{2p_y}^2 \sigma_{2p_z}^2 \overset{*}{\pi}_{2p_x}^1$

$N_b = 10$, $N_a = 5$

$\boxed{\text{Bond order}}$ $B.O. = \frac{1}{2} \times (N_b - N_a)$

$= \frac{1}{2} \times (105)$

$= \frac{1}{2} \times 5 = 2.5$

Bond order for N_2^+ $= 2.5$

$\boxed{\text{Magnetic behaviour}}$:- It has one unpaired electron in $\overset{*}{\pi}_{2p_x}$ molecular orbital

Hence it is $\boxed{\text{paramagnetic}}$ in nature.

④ Electronic configuration of $\underset{(16e^-)}{N_2^{2-}}$ is $\sigma_{1s}^2 \overset{*}{\sigma}_{1s}^2 \sigma_{2s}^2 \overset{*}{\sigma}_{2s}^2 \pi_{2p_x}^2 = \pi_{2p_y}^2 \sigma_{2p_z}^2 \overset{*}{\pi}_{2p_x}^1 = \overset{*}{\pi}_{2p_y}^1$

$N_b = 10$ $N_a = 6$

$B.O = \frac{1}{2} \times (N_b - N_a) = \frac{1}{2} \times (10-6) = \frac{4}{2} = 2$

Bond order for N_2^{2-} is 2

Magnetic character → It has two unpaired electron in each π_{2p_x} and π_{2p_y} molecular orbital.

∴ N_2^{2-} is $\boxed{\text{paramagnetic}}$ in nature.

Molecule	Electronic configuration	Bond order	Magnetic character
N_2	$\sigma_{1s}^2 \sigma_{1s}^{*2} \sigma_{2s}^2 \sigma_{2s}^{*2} \pi_{2p_x}^2 = \pi_{2p_y}^2 \sigma_{2p_z}^2$	$\frac{1}{2} \times (10-4) = \frac{6}{2} = 3$	Diamagnetic
N_2^+	$\sigma_{1s}^2 \sigma_{1s}^{*2} \sigma_{2s}^2 \sigma_{2s}^{*2} \pi_{2p_x}^2 = \pi_{2p_y}^2 \sigma_{2p_z}^1$	$\frac{1}{2} \times (9-4) = \frac{5}{2} = 2.5$	Paramagnetic
N_2^-	$\sigma_{1s}^2 \sigma_{1s}^{*2} \sigma_{2s}^2 \sigma_{2s}^{*2} \pi_{2p_x}^2 = \pi_{2p_y}^2 \sigma_{2p_z}^2 \pi_{2p_x}^{*1}$	$\frac{1}{2} \times (10-5) = 2.5$	Paramagnetic
N_2^{2-}	$\sigma_{1s}^2 \sigma_{1s}^{*2} \sigma_{2s}^2 \sigma_{2s}^{*2} \pi_{2p_x}^2 = \pi_{2p_y}^2 \sigma_{2p_z}^2 \pi_{2p_x}^{*1} = \pi_{2p_y}^{*1}$	$\frac{1}{2} \times (10-6) = 2$	Paramagnetic

Stability order on the basis of Bond order is

$$\boxed{N_2 > (N_2^+ = N_2^-) > N_2^{2-}}$$

Bond order value is higher then stability of molecule will be higher.

$$\boxed{\text{Bond order} \propto \text{Stability}}$$

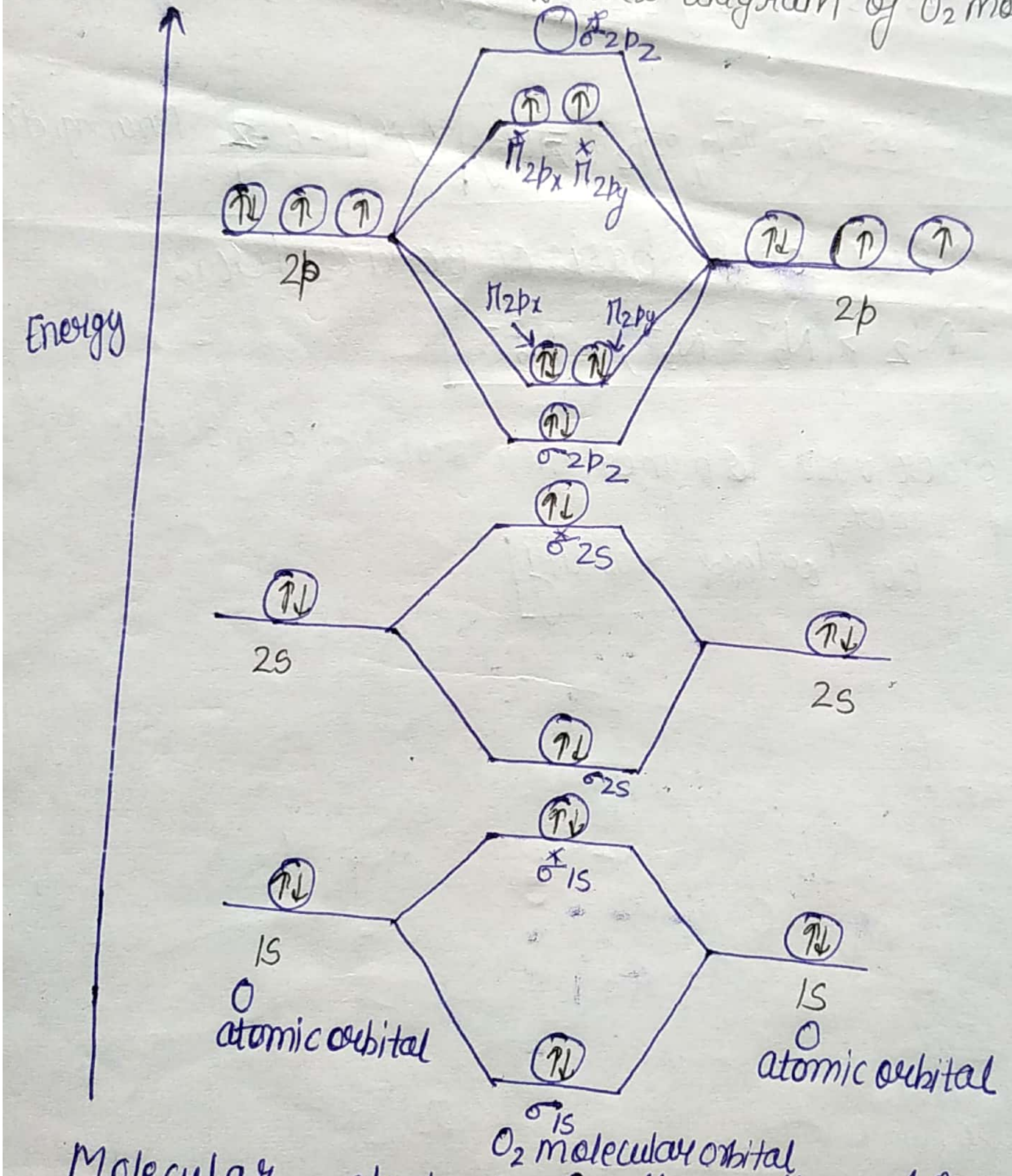
O_2 molecule

Each O atom has 8 electrons and its electronic configuration is $1s^2\ 2s^2\ 2p^4$

Two oxygen atoms overlap to form O_2 molecule.

Total of 16 electrons are then filled in molecular orbitals of O_2 molecule.

Energy level diagram of O_2 molecule



Molecular electronic configuration of O_2 is

$$\sigma_{1s}^2\ \sigma^{*2}_{1s}\ \sigma_{2s}^2\ \sigma^{*2}_{2s}\ \sigma_{2p_z}^2\ \pi_{2p_x}^2 = \pi_{2p_y}^2\ \pi^{*1}_{2p_x} = \pi^{*1}_{2p_y}$$

Bond order : $\frac{1}{2} \times (N_b - N_a)$

$N_b = 10$ → No. of electrons in Bonding molecular orbitals

$N_a = 6$ → No. of electrons in Antibonding molecular orbitals.

$B.O = \frac{1}{2} \times (10-6) = \frac{1}{2} \times 4 = 2$

Bond order of O_2 molecule is $\boxed{2}$

Magnetic character :- O_2 has <u>two unpaired electron</u> in each $\pi^*_{2p_x}$ and $\pi^*_{2p_y}$ orbital.

∴ O_2 is $\boxed{\text{paramagnetic}}$ in <u>nature</u>.

Q. Write the electronic configuration of O_2, O_2^+, O_2^-, O_2^{2-}. Establish their stability order based on calculation of bond order. Also write their magnetic character.

① Electronic configuration of $\underset{(16e^-)}{O_2} = \sigma_{1s}^2 \overset{*}{\sigma}{}_{1s}^2 \sigma_{2s}^2 \overset{*}{\sigma}{}_{2s}^2 \sigma_{2p_z}^2 \pi_{2p_x}^2 = \pi_{2p_y}^2$
$\overset{*}{\pi}{}_{2p_x}^1 = \overset{*}{\pi}{}_{2p_y}^1$

Bond order $= \frac{1}{2} \times (N_b - N_a)$, $N_b = 10$ $N_a = 6$

$= \frac{1}{2} \times (10-6) = \frac{4}{2} = 2$

B.O of $O_2 = 2$

Magnetic character → Two unpaired electrons present in each $\pi^*_{2p_x}$ and $\pi^*_{2p_y}$ orbital

∴ O_2 is $\boxed{\text{paramagnetic}}$ in nature.

② Electronic Configuration of O_2^+ $(15e^-)$ is $\sigma_{1s}^2 \overset{*}{\sigma}_{1s}^2 \sigma_{2s}^2 \overset{*}{\sigma}_{2s}^2 \sigma_{2p_z}^2 \pi_{2p_x} = \pi_{2p_y}^2 \overset{*}{\pi}_{2p_x}^1$

$B\cdot O = \frac{1}{2} \times (N_b - N_a)$ $N_b = 10$, $N_a = 5$

$B\cdot O = \frac{1}{2} \times (10-5) = 2\cdot5$

Bond order for O_2^+ is $\boxed{2\cdot5}$

Magnetic character :- It has one unpaired electron in $\overset{*}{\pi}_{2p_x}$ molecular orbital

O_2^+ is paramagnetic in nature.

③ Electronic configuration of O_2^- $(17e^-)$ is

$\sigma_{1s}^2 \overset{*}{\sigma}_{1s}^2 \sigma_{2s}^2 \overset{*}{\sigma}_{2s}^2 \sigma_{2p_z}^2 \pi_{2p_x}^2 = \pi_{2p_y}^2 \overset{*}{\pi}_{2p_x}^2 = \overset{*}{\pi}_{2p_y}^1$

$N_b = 10$ $N_a = 7$

Bondorder $= \frac{1}{2} \times (10-7) = \frac{3}{2} = 1\cdot5$

Magnetic character :- It has one unpaired electron in $\overset{*}{\pi}_{2p_y}$ molecular orbital.

∴ O_2^- is paramagnetic in nature

④ Electronic configuration of O_2^{2-} (18 electrons) is

$\sigma_{1s}^2 \overset{*}{\sigma}_{1s}^2 \sigma_{2s}^2 \overset{*}{\sigma}_{2s}^2 \sigma_{2p_z}^2 \pi_{2p_x}^2 = \pi_{2p_y}^2 \overset{*}{\pi}_{2p_x}^2 = \overset{*}{\pi}_{2p_y}^2$

$N_b = 10$ $N_a = 8$

Bond order $= \frac{1}{2} \times (10-8) = \frac{2}{2} = 1$

Magnetic character → It has no any unpaired electron in molecular orbital.

∴ O_2^{2-} is diamagnetic in nature

Molecule	No. of electrons	Electronic Configuration	Bond order	Magnetic behaviour
O_2^+	15	$\sigma_{1s}^2, \overset{*}{\sigma}_{1s}^2, \sigma_{2s}^2, \overset{*}{\sigma}_{2s}^2, \sigma_{2p_z}^2, \pi_{2p_x}^2 = \pi_{2p_y}^2\ \overset{*}{\pi}_{2p_x}^1$	2.5	Paramagnetic
O_2	16	$\sigma_{1s}^2 \overset{*}{\sigma}_{1s}^2 \sigma_{2s}^2 \overset{*}{\sigma}_{2s}^2\ \sigma_{2p_z}^2\ \pi_{2p_x}^2 = \pi_{2p_y}^2\ \overset{*}{\pi}_{2p_x}^1 = \overset{*}{\pi}_{2p_y}^1$	2	Paramagnetic
O_2^-	17	$\sigma_{1s}^2 \overset{*}{\sigma}_{1s}^2 \sigma_{2s}^2 \overset{*}{\sigma}_{2s}^2\ \sigma_{2p_z}^2\ \pi_{2p_x}^2 = \pi_{2p_y}^2\ \overset{*}{\pi}_{2p_x}^2 = \overset{*}{\pi}_{2p_y}^1$	1.5	Paramagnetic
O_2^{2-}	18	$\sigma_{1s}^2 \overset{*}{\sigma}_{1s}^2 \sigma_{2s}^2 \overset{*}{\sigma}_{2s}^2\ \sigma_{2p_z}^2\ \pi_{2p_x}^2 = \pi_{2p_y}^2\ \overset{*}{\pi}_{2p_x}^2 = \overset{*}{\pi}_{2p_y}^2$	1	Diamagnetic

Bond order → $\boxed{O_2^+ > O_2 > O_2^- > O_2^{2-}}$

Bond dissociation energy → Bond order value is higher, more will be bond dissociation energy.

∴ order for bond dissociation energy ⇒ $\boxed{O_2^+ > O_2 > O_2^- > O_2^{2-}}$

- F_2 molecule

F atom has 9 electrons and it has electronic configuration is $1s^2\ 2s^2\ 2p^5$. Two fluorine atoms overlap to form F_2 molecule. Total of 18 electrons are then filled in molecular orbitals of F_2 molecule.

Molecular Orbital electronic configuration of F_2 is

$$\sigma_{1s}^2\ \overset{*}{\sigma}_{1s}^2\ \sigma_{2s}^2\ \overset{*}{\sigma}_{2s}^2\ \sigma_{2p_z}^2\ \pi_{2p_x}^2 = \pi_{2p_y}^2\ \ \overset{*}{\pi}_{2p_x}^2 = \overset{*}{\pi}_{2p_y}^2$$

$N_b = 10 \quad N_a = 8$

Bond order $= \frac{1}{2} \times (N_b - N_a)$

N_b = no. of e^- in Bonding molecular orbital

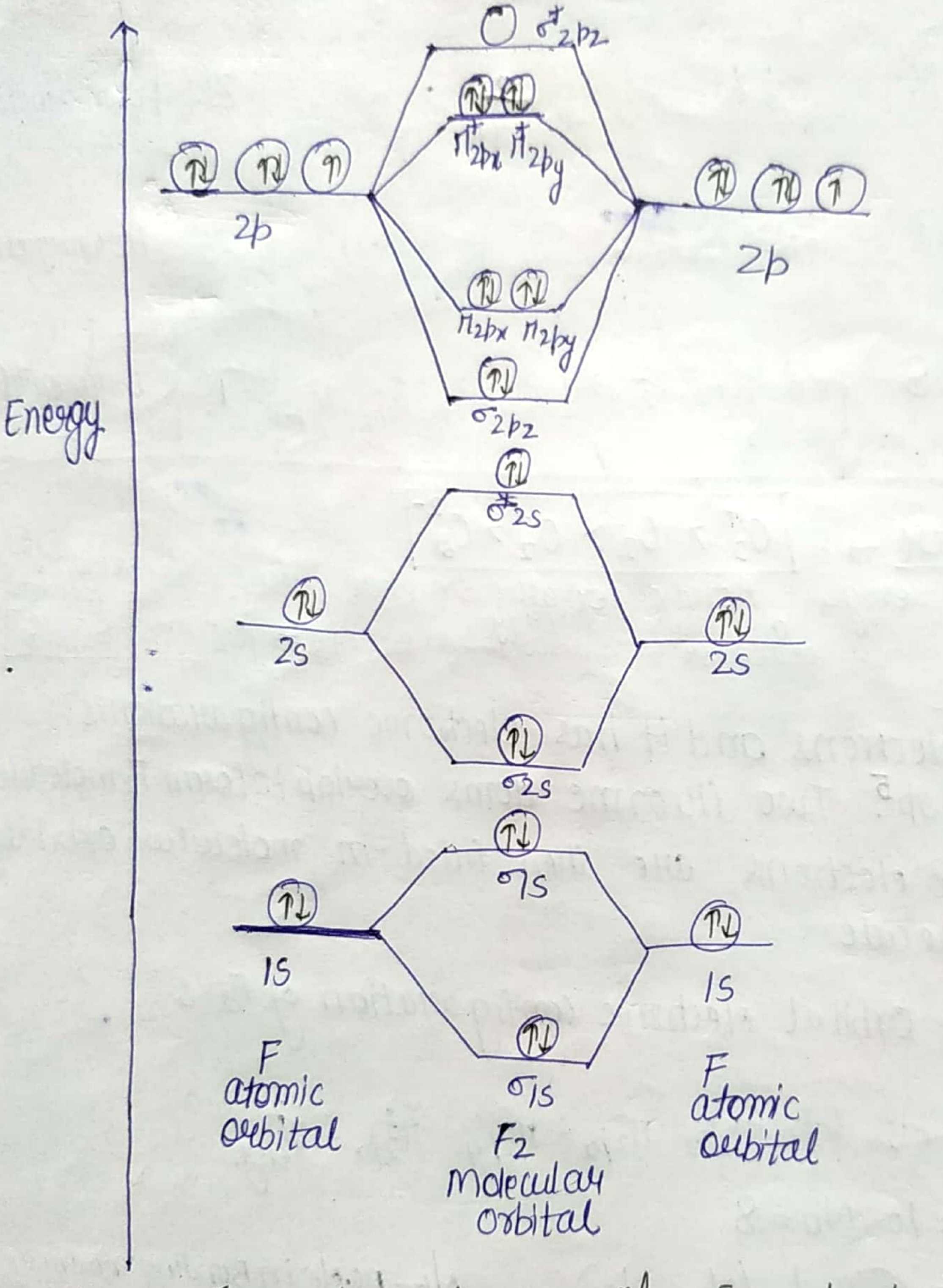
N_a = no. of e^- in Antibonding molecular orbital

$= \frac{1}{2} \times (10 - 8) = \frac{2}{2} = 1$

$\boxed{\text{Bond order of } F_2 \text{ is } 1}$

Magnetic behaviour:- It has no any unpaired electrons in molecular orbital.

∴ F_2 is $\boxed{\text{diamagnetic}}$ in nature.



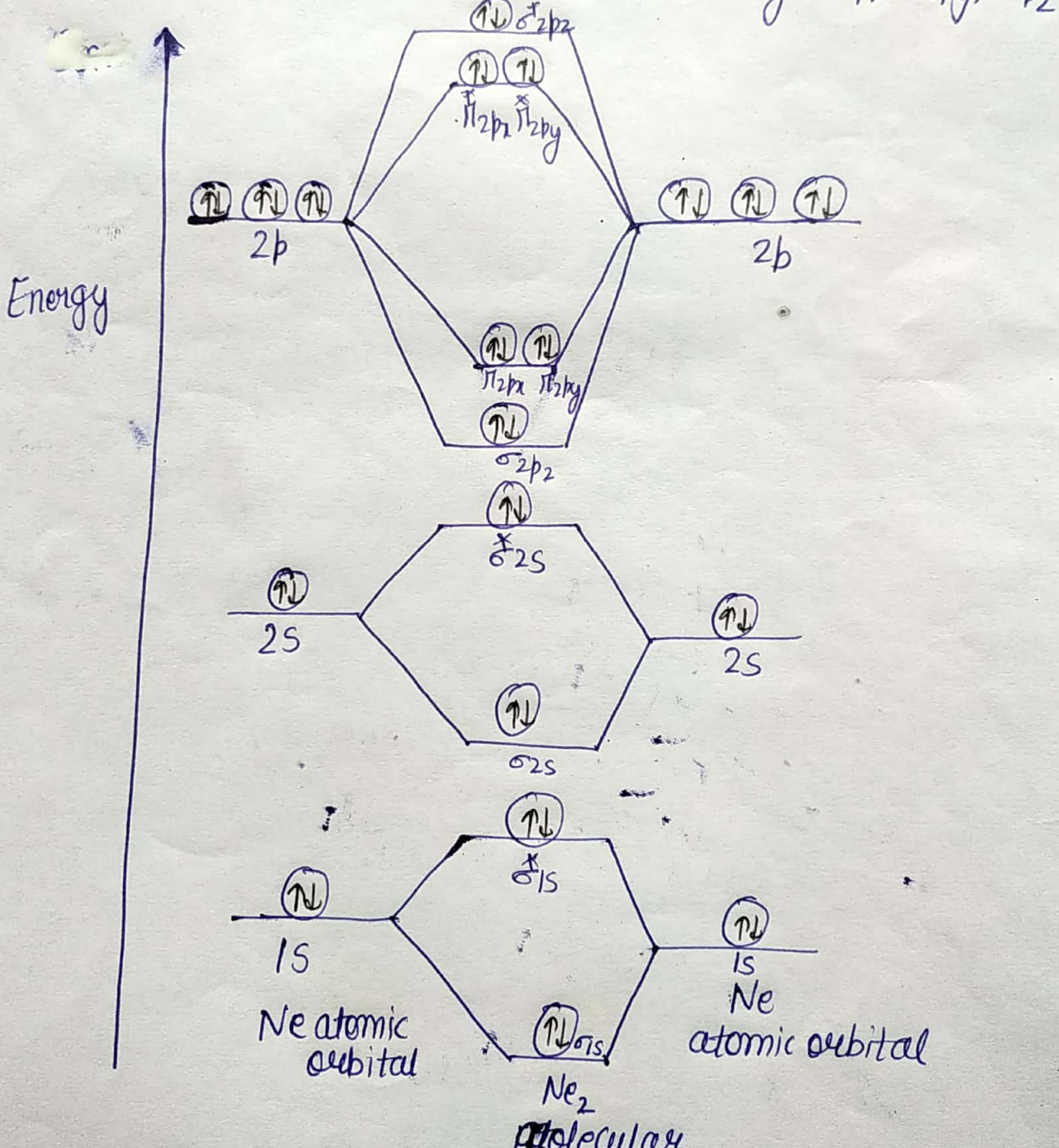
Energy level diagram of F_2 molecule

Ne_2 molecule

Ne has 10 electrons and its electronic configuration is $1s^2\ 2s^2\ 2p^6$

Two Ne atoms overlap to form Ne_2 molecule. Total of 20 electrons are then filled in molecular orbitals of Ne_2 molecule.

$\sigma_{1s}^2\ \overset{*}{\sigma}{}_{1s}^2\ \sigma_{2s}^2\ \overset{*}{\sigma}{}_{2s}^2\ \sigma_{2p_z}^2,\ \pi_{2p_x}^2 = \pi_{2p_y}^2,\ \overset{*}{\pi}{}_{2p_x}^2 = \overset{*}{\pi}{}_{2p_y}^2,\ \overset{*}{\sigma}{}_{2p_z}^2$



Energy level diagram of Ne_2

Bond order $= \frac{1}{2} \times (N_b - N_a) = \frac{1}{2}(10-10) = 0 \rightarrow \therefore Ne_2$ does not exist

Energy level Diagram for Heteronuclear Diatomic molecule

① NO molecule

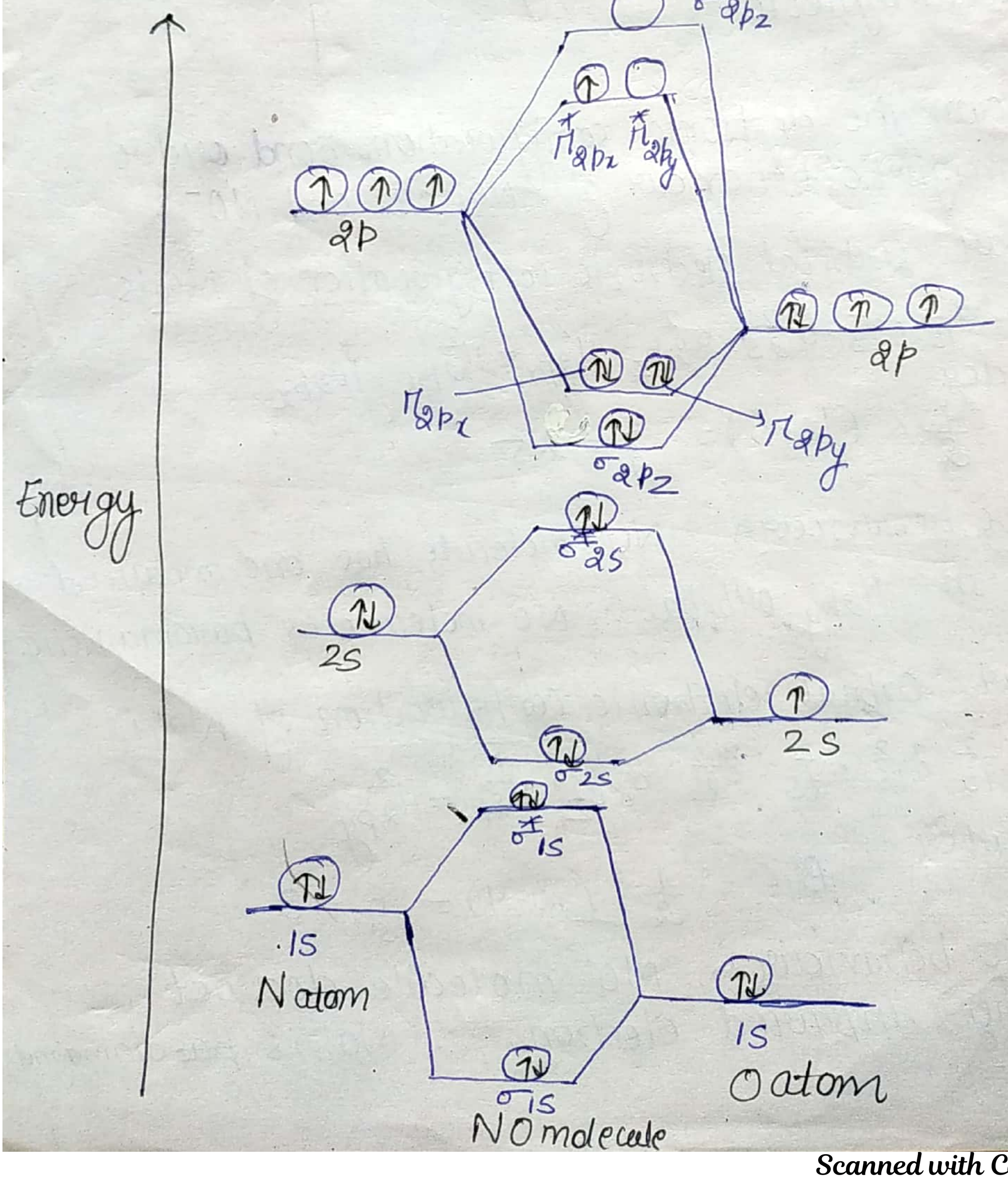
Nitrogen atom has 7 electrons and its configuration is $1s^2 2s^2 2p^3$

Oxygen atom has 8 electrons and its configuration is $1s^2 2s^2 2p^4$

∴ NO molecule has 15 electrons

① Molecular orbital electronic configuration of No molecule

$\sigma_{1s}^2 \overset{*}{\sigma}{}_{1s}^2 \sigma_{2s}^2 \overset{*}{\sigma}{}_{2s}^2 \sigma_{2p_z}^2 \pi_{2p_x}^2 = \pi_{2p_y}^2 \overset{*}{\pi}{}_{2p_x}^1$



② Bond order $= \frac{1}{2} \times$ (Number of electrons in Bonding molecular orbital − Number of electrons in Antibonding molecular orbital)

$$B.O = \frac{1}{2} \times (N_b - N_a)$$

$N_b = 10 \quad N_a = 5$

$$B.O = \frac{1}{2} \times (10-5) = \frac{5}{2} = 2.5$$

③ Magnetic character → **NO** molecule contains one unpaired electron in π^{*}_{2py} orbital ∴ <u>NO</u> molecule is para magnetic.

Write down the electronic configuration, bond order and magnetic behaviour of NO NO⁺ and NO⁻

① <u>Molecular Orbital electronic configuration of NO is</u>

$$\sigma^2_{1s}\ \sigma^{*2}_{1s}\ \sigma^2_{2s}\ \sigma^{*2}_{2s}\ \sigma^2_{2p_z}\ \pi^2_{2p_x} = \pi^2_{2p_y}\ \pi^{*1}_{2p_x}$$

<u>Bond order</u>

$$B.O = \frac{1}{2} \times (10-5) = \frac{5}{2} = 2.5$$

<u>Magnetic behaviour</u> → NO molecule has one unpaired electron in $\pi^{*}_{2p_y}$ orbital ∴ NO molecule is paramagnetic.

② <u>Molecular Orbital electronic configuration of NO⁺ is</u>

$$\sigma^2_{1s}\ \sigma^{*2}_{1s}\ \sigma^2_{2s}\ \sigma^{*2}_{2s}\ \sigma^2_{2p_z}\ \pi^2_{2p_x} = \pi^2_{2p_y}$$

<u>Bond order</u>

$$B.O = \frac{1}{2} \times (10-4) = \frac{6}{2} = 3$$

<u>Magnetic behaviour</u> → NO⁺ molecule does not has any unpaired electron. ∴ NO⁺ is ~~par~~ diamagnetic

③ Molecular orbital electronic configuration of NO^- is

$$\sigma_{1s}^2 \, \overset{*}{\sigma}{}_{1s}^2 \, \sigma_{2s}^2 \, \overset{*}{\sigma}{}_{2s}^2 \, \sigma_{2p_z}^2 \, \pi_{2p_x}^2 = \pi_{2p_y}^2 \, \overset{*}{\pi}{}_{2p_x}^1 = \overset{*}{\pi}{}_{2p_y}^1$$

Bond order

$$B.O = \frac{1}{2} \times (10-6) = \frac{4}{2} = 2$$

Magnetic behaviour → NO^- molecule has two unpaired electron, one in $\overset{*}{\pi}_{2p_x}$ and another in $\overset{*}{\pi}_{2p_y}$ ∴ NO^- is paramagnetic.

Molecule	Electronic Configuration	Bond Order	Magnetic Behaviour
NO	$\sigma_{1s}^2 \overset{*}{\sigma}{}_{1s}^2 \sigma_{2s}^2 \overset{*}{\sigma}{}_{2s}^2 \sigma_{2p_z}^2 \pi_{2p_x}^2 = \pi_{2p_y}^2 \overset{*}{\pi}{}_{2p_x}^1$	$\frac{1}{2} \times (10-5) = 2.5$	Paramagnetic
NO^+	$\sigma_{1s}^2 \overset{*}{\sigma}{}_{1s}^2 \sigma_{2s}^2 \overset{*}{\sigma}{}_{2s}^2 \sigma_{2p_z}^2 \pi_{2p_x}^2 = \pi_{2p_y}^2$	$\frac{1}{2} \times (10-4) = 3$	Diamagnetic
NO^-	$\sigma_{1s}^2 \overset{*}{\sigma}{}_{1s}^2 \sigma_{2s}^2 \overset{*}{\sigma}{}_{2s}^2 \sigma_{2p_z}^2 \pi_{2p_x}^2 = \pi_{2p_y}^2$ $\overset{*}{\pi}{}_{2p_x}^1 = \overset{*}{\pi}{}_{2p_y}^1$	$\frac{1}{2} \times (10-6) = 2$	Paramagnetic

Stability order

Higher the Bond order value more will be stability of molecule → $\boxed{\text{Bond order of } NO^+ > B.O \text{ of } NO > B.O \text{ of } NO^-}$

∴ stability order is

$$\boxed{\therefore \; NO^+ > NO > NO^-}$$

② CN molecule

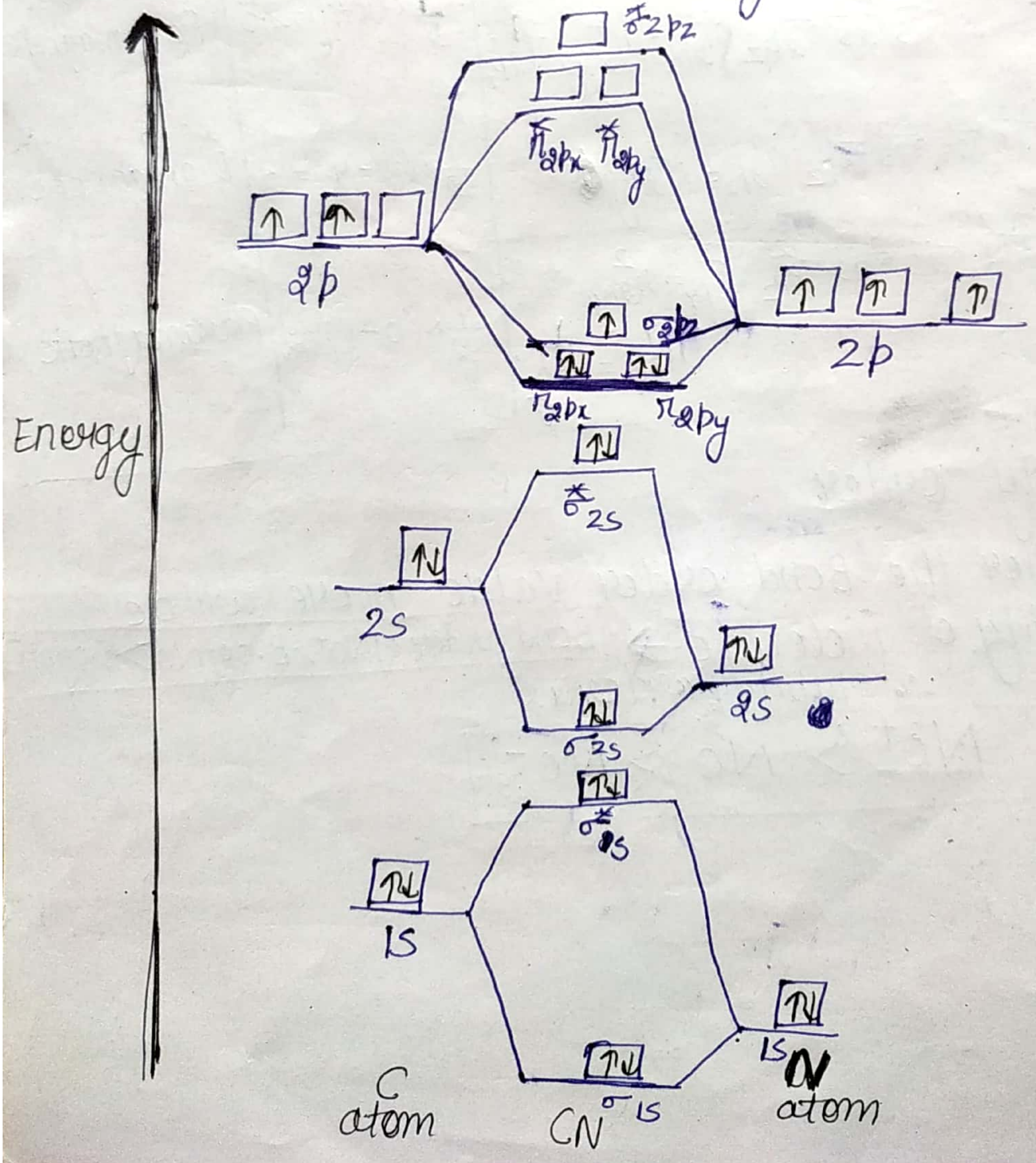
Carbon atom has 6 electrons and its configuration is $1s^2 2s^2 2p^2$

Nitrogen atom has 7 electrons and its configuration is $1s^2 2s^2 2p^3$

∴ CN molecule has 13 electrons

ⓐ Molecular orbital electronic configuration of CN molecule

$$\sigma_{1s}^2 \overset{*}{\sigma}{}_{1s}^2 \sigma_{2s}^2 \overset{*}{\sigma}{}_{2s}^2 \pi_{2p_x}^2 = \pi_{2p_y}^2 \sigma_{2p_z}^1$$



ⓑ Bond order $= \frac{1}{2} \times \left(\text{Number of electrons in Bonding molecular orbital} - \text{Number of electrons in Antibonding molecular orbital} \right)$

$$B.O = \frac{1}{2} \times (N_b - N_a)$$

$$N_b = 9 \quad N_a = 4$$

$$B.O = \frac{1}{2} \times (9-4) = \frac{5}{2} = 2.5$$

ⓒ Magnetic behaviour → CN molecule has one unpaired electron in σ_{2p_z} orbital. Therefore CN is paramagnetic in nature.

Write down the electronic configuration, bond order and magnetic behaviour of CN^-.

Carbon atom has 6 electrons

Its configuration is $1s^2 2s^2 2p^2$

Nitrogen atom has 7 electrons

Its configuration is $1s^2 2s^2 2p^3$

∴ CN^- molecule has $6+7+1 = 14$ electrons

Electronic configuration of CN^- is

$$\sigma_{1s}^2 \overset{*}{\sigma}_{1s}^2 \; \sigma_{2s}^2 \overset{*}{\sigma}_{2s}^2 \; \pi_{2p_x}^2 = \pi_{2p_y}^2 \; \sigma_{2p_z}^2$$

Bond order $= \frac{1}{2} \left(\text{No. of electrons in Bonding molecular orbital} - \text{Number of electrons in Antibonding molecular orbital} \right)$

$$B.O = \frac{1}{2} (N_b - N_a)$$

~~Electronic~~ $B.O = \frac{1}{2} \times (10-4) = \frac{6}{2} = 3$

Magnetic behaviour → CN^- is diamagnetic because it does not have any unpaired electron.

CO molecule

Carbon atom has 6 electrons

Electronic configuration of Carbon atom is $1s^2 2s^2 2p^2$

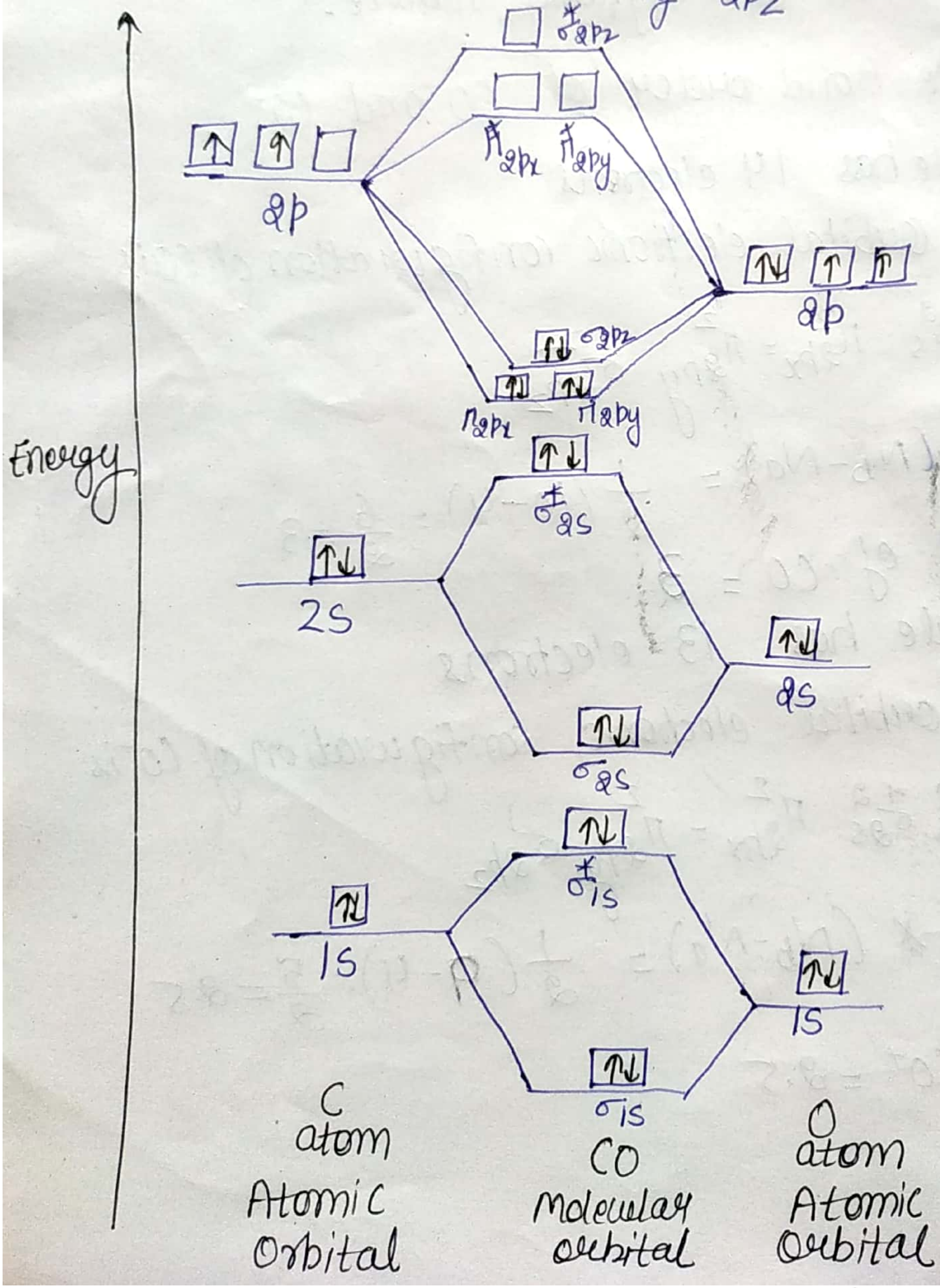
Oxygen atom has 8 electrons

Electronic configuration of Oxygen atom is $1s^2 2s^2 2p^4$

∴ CO molecule has 14 electrons.

a) Molecular orbital electronic configuration of CO molecule

$\sigma_{1s}^2 \; \overset{*}{\sigma}{}_{1s}^2 \; \sigma_{2s}^2 \; \overset{*}{\sigma}{}_{2s}^2 \; \pi_{2p_x}^2 = \pi_{2p_y}^2 \; \sigma_{2p_z}^2$



Bond order $= \frac{1}{2} \times$ (Number of electrons in Bonding molecular orbital − Number of electrons in Anti bonding molecular orbital)

$$B.O = \frac{1}{2} \times (N_b - N_a)$$

$$N_b = \frac{1}{2} \times (10-4) \Rightarrow \frac{6}{2} = 3 \Rightarrow \boxed{C \equiv O}$$

Magnetic Behaviour → CO molecule has no. unpaired electrons. Therefore CO is diamagnetic nature.

Calculate the Bond order of CO and CO^+

CO molecule has 14 electrons

Molecular Orbital electronic configuration of CO is

$$\sigma_{1s}^2 \, \sigma_{1s}^{*2} \, \sigma_{2s}^2 \, \sigma_{2s}^{*2} \, \pi_{2p_x}^2 = \pi_{2p_y}^2 \, \sigma_{2p_z}^2$$

$$B.O = \frac{1}{2} \times (N_b - N_a) = \frac{1}{2}(10-4) = \frac{6}{2} = 3$$

B.O of CO = 3

CO^+ molecule has 13 electrons

Molecular orbital electronic configuration of CO^+ is

$$\sigma_{1s}^2 \, \sigma_{1s}^{*2} \, \sigma_{2s}^2 \, \sigma_{2s}^{*2} \, \pi_{2p_x}^2 = \pi_{2p_y}^2 \, \sigma_{2p_z}^1$$

$$B.O = \frac{1}{2} \times (N_b - N_a) = \frac{1}{2}(9-4) = \frac{5}{2} = 2.5$$

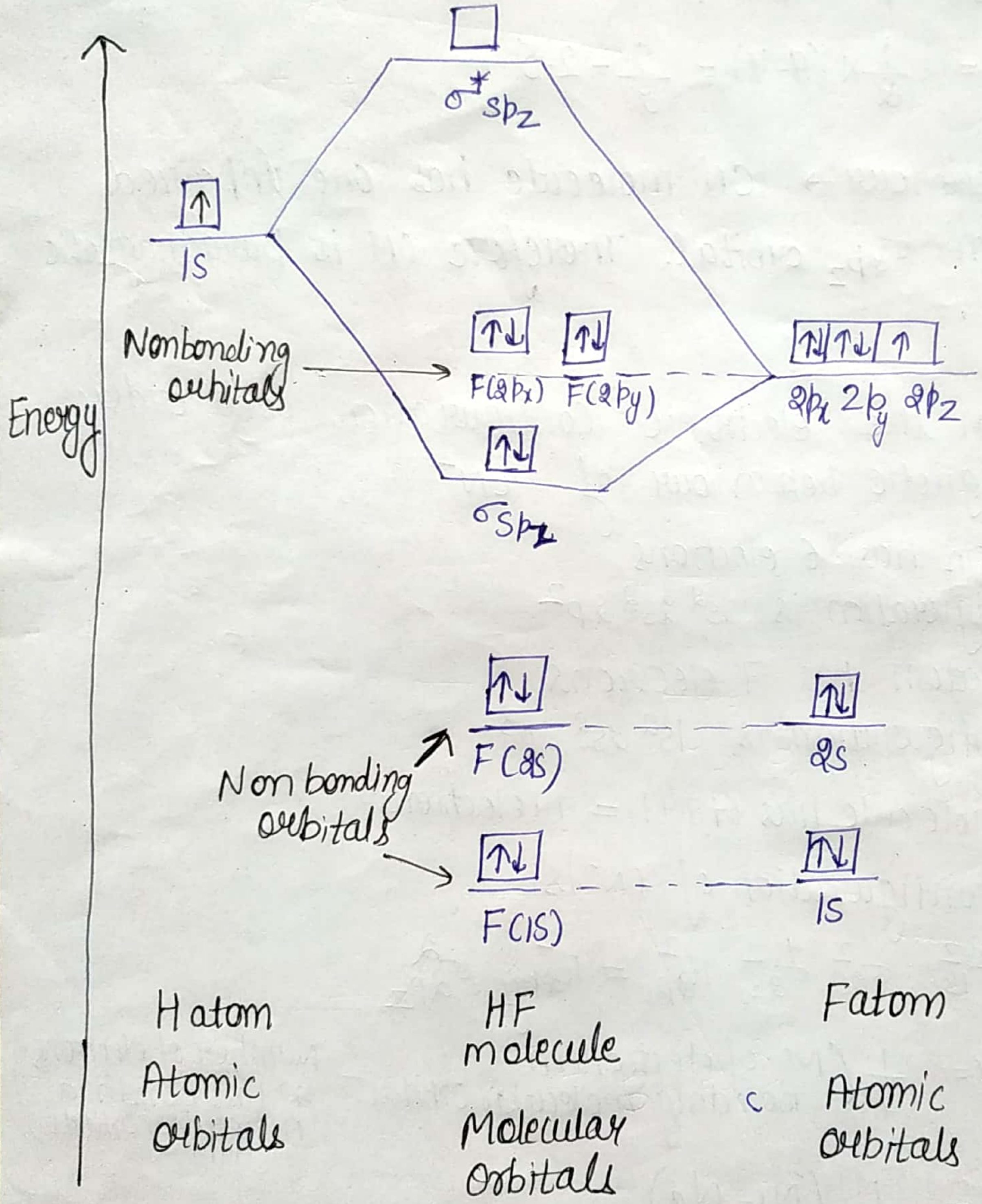
B.O of CO^+ = 2.5

HF molecule

H atom has 1electron. and its configuration is $1s^1$

Fluorine atom has 9 electrons and its configuration is $1s^2 2s^2 2p^5$

∴ HF molecule has 10 electrons.



Molecular orbital electronic configuration of HF molecule is

$$1s^2\ 2s^2\ \sigma sp_z^2\ \ 2p_x^2 = 2p_y^2$$

Bond order of HF molecule

$$= \frac{1}{2} \times (N_b - N_a)$$

$$= \frac{1}{2} \times (2-0) = 1$$

Magnetic behaviour → All molecular orbitals are combletely filled. Hence HF molecule is diamagnetic.

Nonbonding molecular orbitals

A nonbonding orbital is a molecular orbital for which addition or removal of an electron does not change the energy of molecule.

e.g. HF has 10 electrons

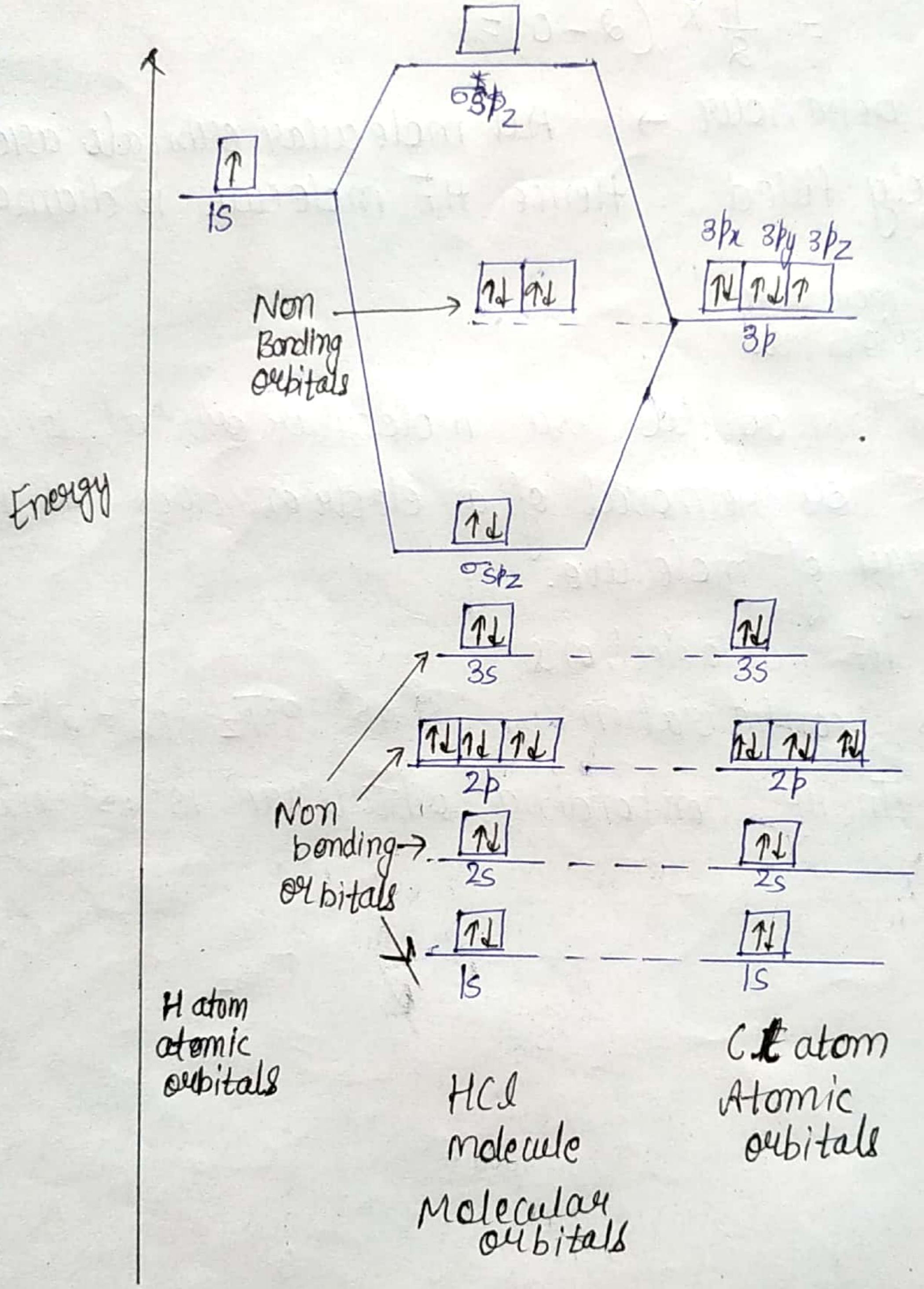
its configuration is $1s^2\ 2s^2\ \sigma^2_{sp_z}\ 2p_x^2 = 2p_y^2$

In HF, nonbonding orbitals are $1s^2\ 2s^2\ 2p_x^2 = 2p_y^2$

HCl molecule

→ H atom has 1 electron and its configuration is $1s^1$

→ Cl atom has 17 electrons andits configuration is $1s^2 2s^2 2p^6 3s^2 3p^5$



Molecular orbital electronic configuration of HCl moleculeis

$1s^2\ 2s^2\ 2p^6\ 3s^2\ \sigma_{sp_z}^2\ 3p_x^2 = 3p_y^2$

Bond Order of HCl molecule

$$= \frac{1}{2} \times (N_b - N_a)$$

$$= \frac{1}{2} \times (2-0) = 1$$

Bond order of HCl molecule is 1.

∴ There is single bond btw H and Cl atoms.

Magnetic behaviour →

All molecular orbitals are completely filled.

Hence HCl molecule is diamagnetic.

Energy level diagram for $\boxed{NO^+}$ molecule

Nitrogen atom has 7 electrons & its configuration is $1s^2 2s^2 2p^3$

Oxygen atom has 8 electrons & its configuration is $1s^2 2s^2 2p^4$

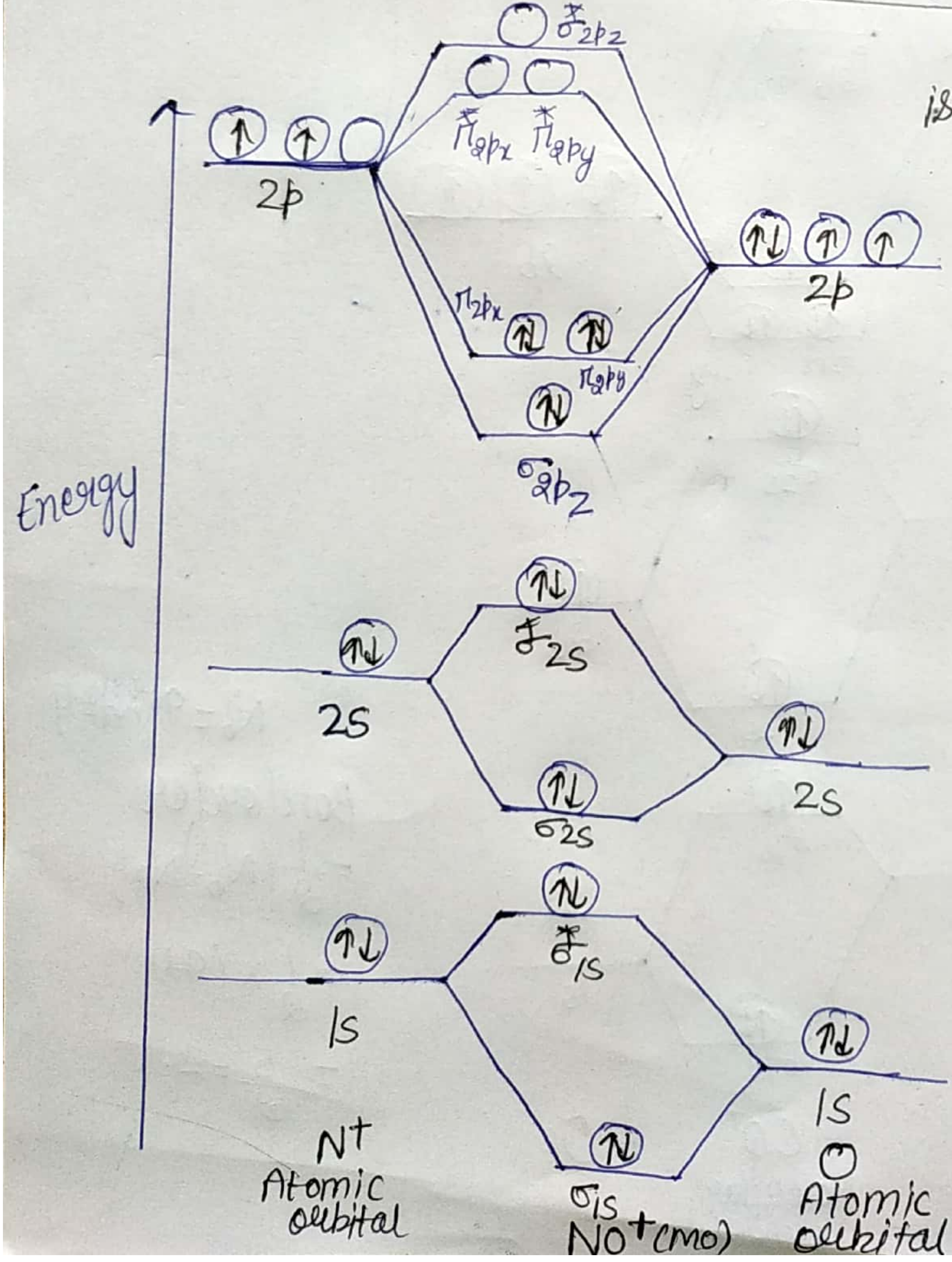
∴ NO molecule has 15 electrons & configuration for NO molecule is $\sigma_{1s}^2 \overset{*}{\sigma}_{1s}^2 \sigma_{2s}^2 \overset{*}{\sigma}_{2s}^2 \sigma_{2p_z}^2 \pi_{2p_x}^2 = \pi_{2p_y}^2 \overset{*}{\pi}_{2p_x}^1$

NO⁺ molecule has 14 electrons

∴ configuration for NO⁺ should be that which have been followed for NO molecule.

∴ NO⁺ molecule has electronic configuration is

$$\boxed{\sigma_{1s}^2 \overset{*}{\sigma}_{1s}^2 \sigma_{2s}^2 \overset{*}{\sigma}_{2s}^2 \sigma_{2p_z}^2 \pi_{2p_x}^2 = \pi_{2p_y}^2}$$



More ~~less~~ electronegative atom with positive charge is less stable and O is more electronegative than N atom

∴ N will have +ve charge

and hence ~~its~~ N⁺ has configuration $1s^2 2s^2 2p^2$

or

In NO⁺, one electron will be remove from less electronegative atom i.e $\boxed{N}$ atom.

$N_b = 10$ $N_a = 4$

Bond order

$= \frac{1}{2} \times (N_b - N_a)$

$= \frac{1}{2} \times (10 - 4)$

$= 3$

B

Energy level diagram of CO^+

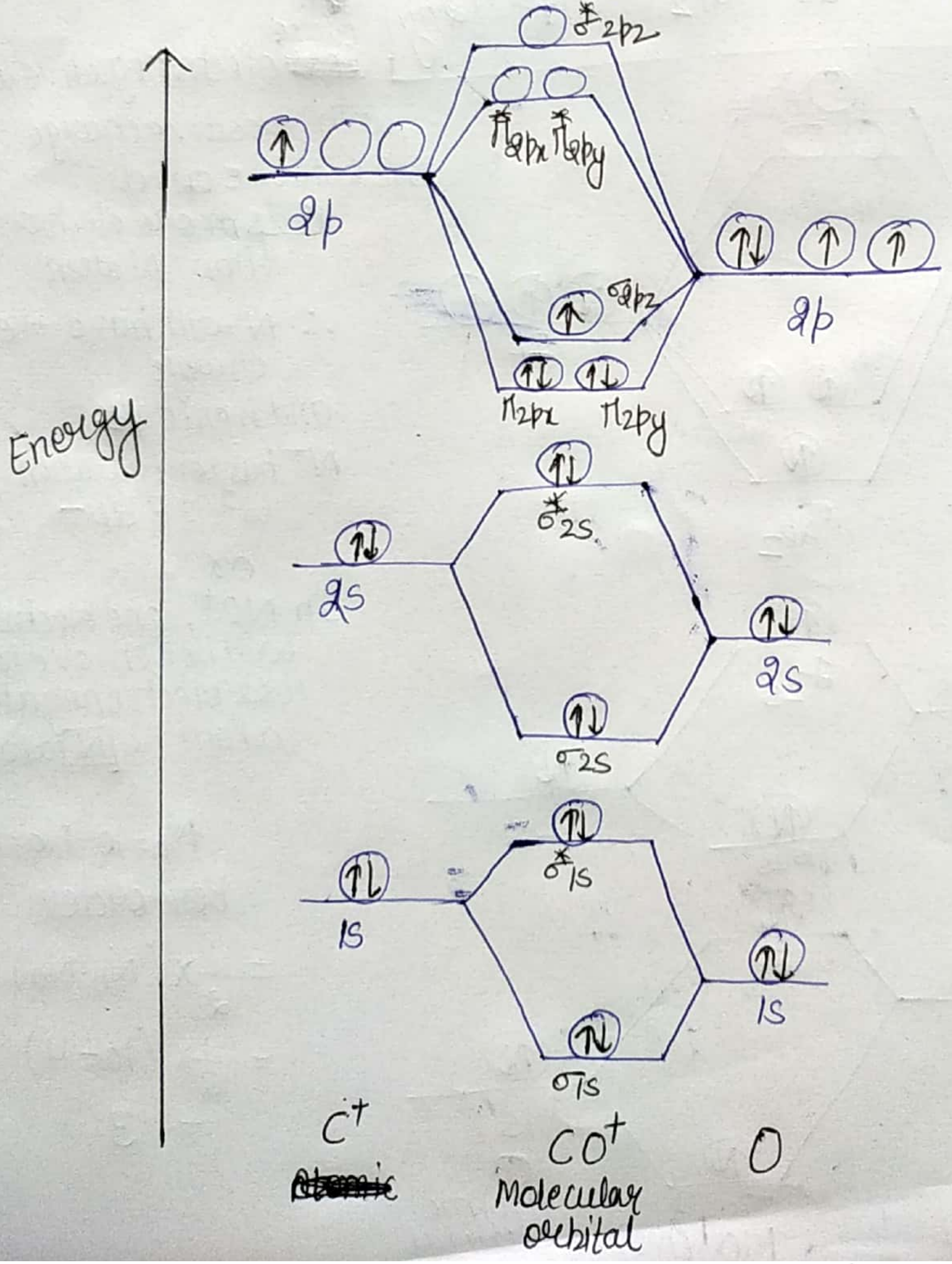
- Carbon atom has 6 electrons and its configuration is $1s^2 2s^2 2p^2$.
- Oxygen atom has 8 electrons and its configuration is $1s^2 2s^2 2p^4$.

∴ CO molecule has 14 electrons.

- Hence CO^+ has 13 electrons.
- CO^+ obtained from removal of one electron ~~and the~~ from CO and that electron is removed from carbon atom because it is less electronegative atom.

∴ configuration of CO^+ → $\boxed{\sigma_{1s}^2 \overset{*}{\sigma}_{1s}^2 \sigma_{2s}^2 \overset{*}{\sigma}_{2s}^2 \pi_{2p_x}^2 = \pi_{2p_y}^2 \sigma_{2p_z}^1}$

∴ In CO^+, carbon present as $C^+ \rightarrow 1s^2 2s^2 2p^1$
$O \rightarrow 1s^2 2s^2 2p^4$
] → combine to form CO^+



$N_b = 9$ $N_a = 4$

Bond order

$= \frac{1}{2}(N_b - N_a)$

$= \frac{1}{2} \times (9-4)$

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

Molecular orbital diagram of CN^-

- Carbon atom has 6 electrons and its configuration is $1s^2 2s^2 2p^2$.
- Nitrogen atom has 7 electrons and its configuration is $1s^2 2s^2 2p^3$.

∴ CN molecule has 13 electrons.

- $CN + e^- \rightarrow CN^- \rightarrow$ CN^- formed by gain of one electron by CN molecule.

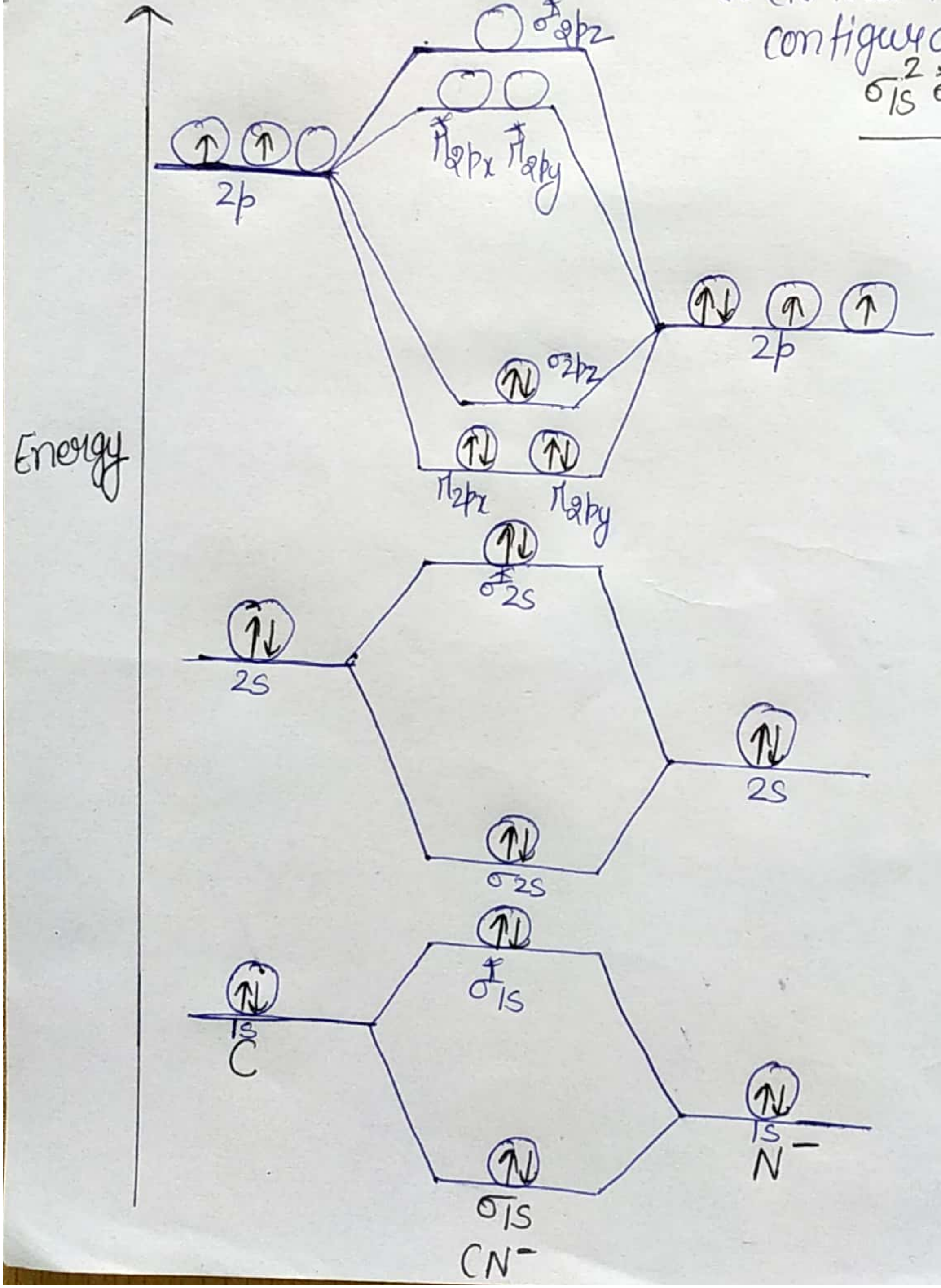
And in CN^-, Nitrogen is present as N^- i.e. -ve charge on nitrogen because it is more electronegative atom.

∴ In $CN^- \rightarrow$ $C \rightarrow 1s^2 2s^2 2p^2$
$N^- \rightarrow 1s^2 2s^2 2p^4$ $\Big]\rightarrow$ combine to form CN⁻ molecule

∴ CN⁻ has 14 electrons

configuration is

$\sigma_{1s}^2 \overset{*}{\sigma}{}_{1s}^2 \sigma_{2s}^2 \overset{*}{\sigma}{}_{2s}^2 \pi_{2px}^2 = \pi_{2py}^2 \sigma_{2pz}^2$



$N_b = 10$ $N_a = 4$

Bond order

$= \frac{1}{2} \times (N_b - N_a)$

$= \frac{1}{2}(10-4) = \frac{6}{2} = 3$

Q→ H forms diatomic molecule while Helium remains mono atomic. Why?

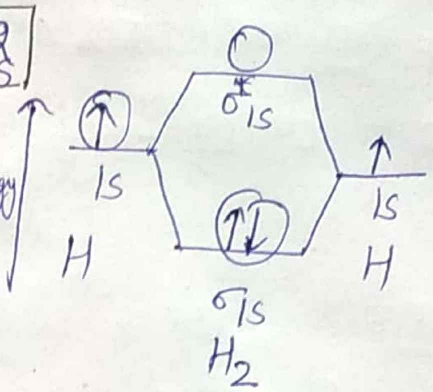
① H as diatomic molecule i.e H_2.

It has $2e^-$ and its configuration is $\boxed{\sigma_{1s}^{2}}$

∴ $\boxed{\text{Bond order} = \frac{1}{2}\times(N_b - N_a)}$

and $N_b = 2$ $N_a = 0$

∴ Bond order $= \frac{1}{2}\times(2-0) = 1$



It means there is single bond between two H atoms.

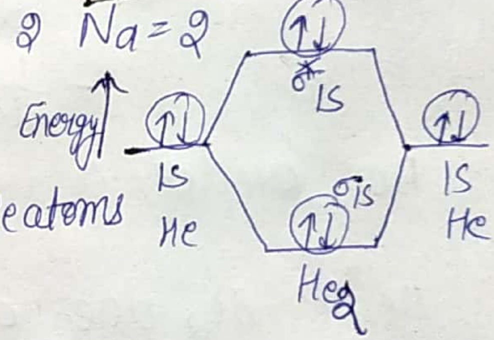
∴ H_2 is stable hence H exist as diatomic molecule.

② He as diatomic molecule i.e He_2

He_2 has 4 electrons and its configuration is $\boxed{\sigma_{1s}^{2}\,\sigma^{*2}_{1s}}$

∴ $\boxed{\text{Bond order} = \frac{1}{2}\times(N_b - N_a)}$ $N_b = 2$ $N_a = 2$

and Bond order $= \frac{1}{2}\times(2-2) = 0$



it means there is no bond between two He atoms

Hence He_2 does not exist.

Therefore He exist as monoatomic

Q→ Li forms diatomic mole cule whereas Beryllium remains monoatomic

1. Li as diatomic molecule ie. Li_2

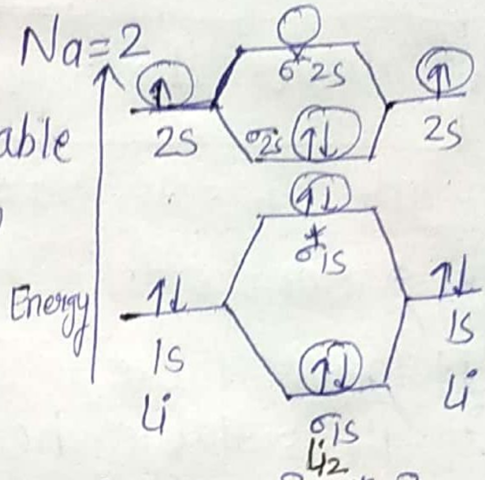
Li_2 has 6 electrons and its configuration is $\sigma_{1s}^2 \overset{*}{\sigma}_{1s}^2 \sigma_{2s}^2$

∴ Bond order = $\frac{1}{2} \times (N_b - N_a)$, $N_b = 4$ $N_a = 2$

$= \frac{1}{2} \times (4-2) = 1$ → Li_2 is stable

It means there is single bond between b/w two Li atoms

Hence Li exist as diatomic molecule



2. Be as diatomic molecule i-e Be_2

Be_2 has 8 electrons and its configuration is $\sigma_{1s}^2 \overset{*}{\sigma}_{1s}^2 \sigma_{2s}^2 \overset{*}{\sigma}_{2s}^2$

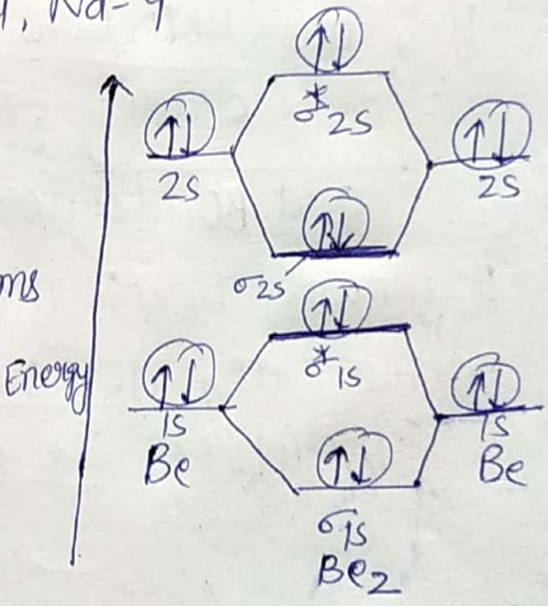
∴ Bond order = $\frac{1}{2} \times (N_b - N_a)$, $N_b = 4$, $N_a = 4$

$= \frac{1}{2} \times (4-4) = 0$

Bond oreder = 0 i.e there is no bond between two Be atoms

Hence Be_2 doesnot exist

∴ Be remains monoatomic



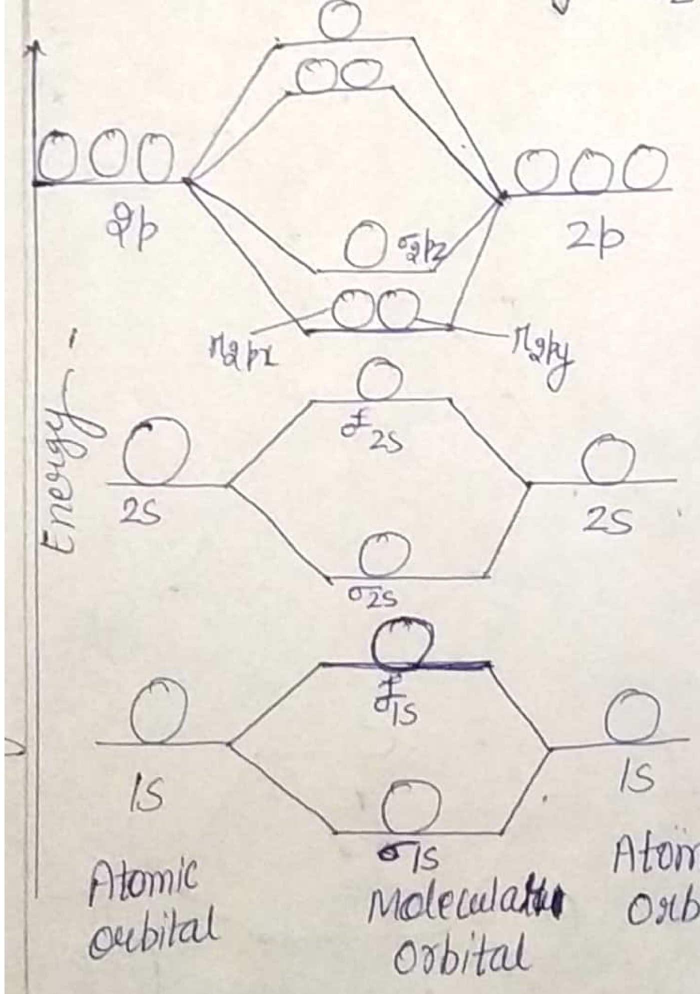
Energy level diagram or Molecular orbital diagram of Homonuclear diatomic molecules

Molecules

① $H_2, H_2^+, H_2^-, H_2^{2-}$
② He_2
③ Li_2
④ Be_2
⑤ B_2
⑥ C_2
⑦ N_2, N_2^+, N_2^-

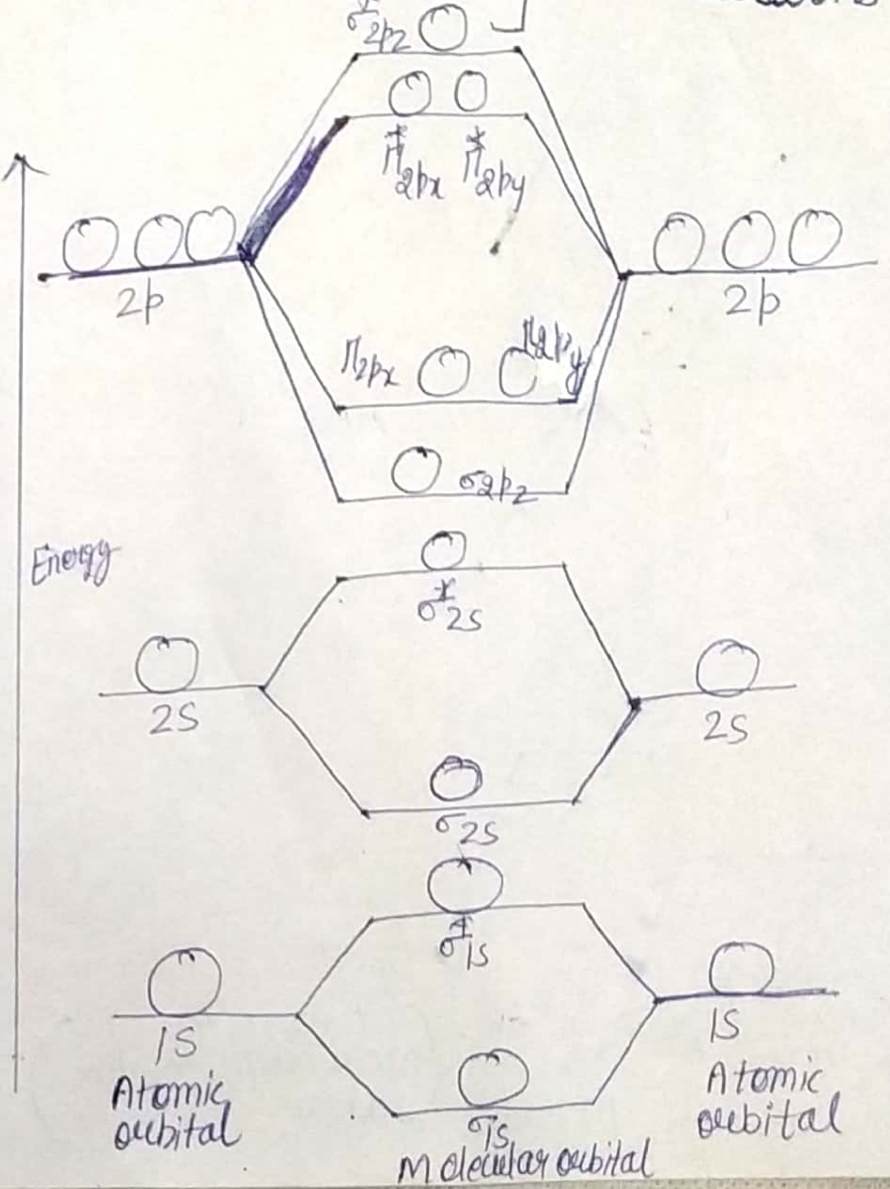
→ $H_2 \to N_2$ this increasing order has to be followed for filling the electrons

$\sigma_{1s}\ \sigma^*_{1s}\ \sigma_{2s}\ \sigma^*_{2s}\ \pi_{2p_x} = \pi_{2p_y}\ \sigma_{2p_z}$
$\pi^*_{2p_x} = \pi^*_{2p_y}\ \sigma^*_{2p_z}$



1. $O_2 \to O_2^+, O_2^-, O_2^{2-}$
2. F_2
3. Ne_2

→ $O_2 \to Ne_2$ increasing order has to be followed for filling the electrons in molecule

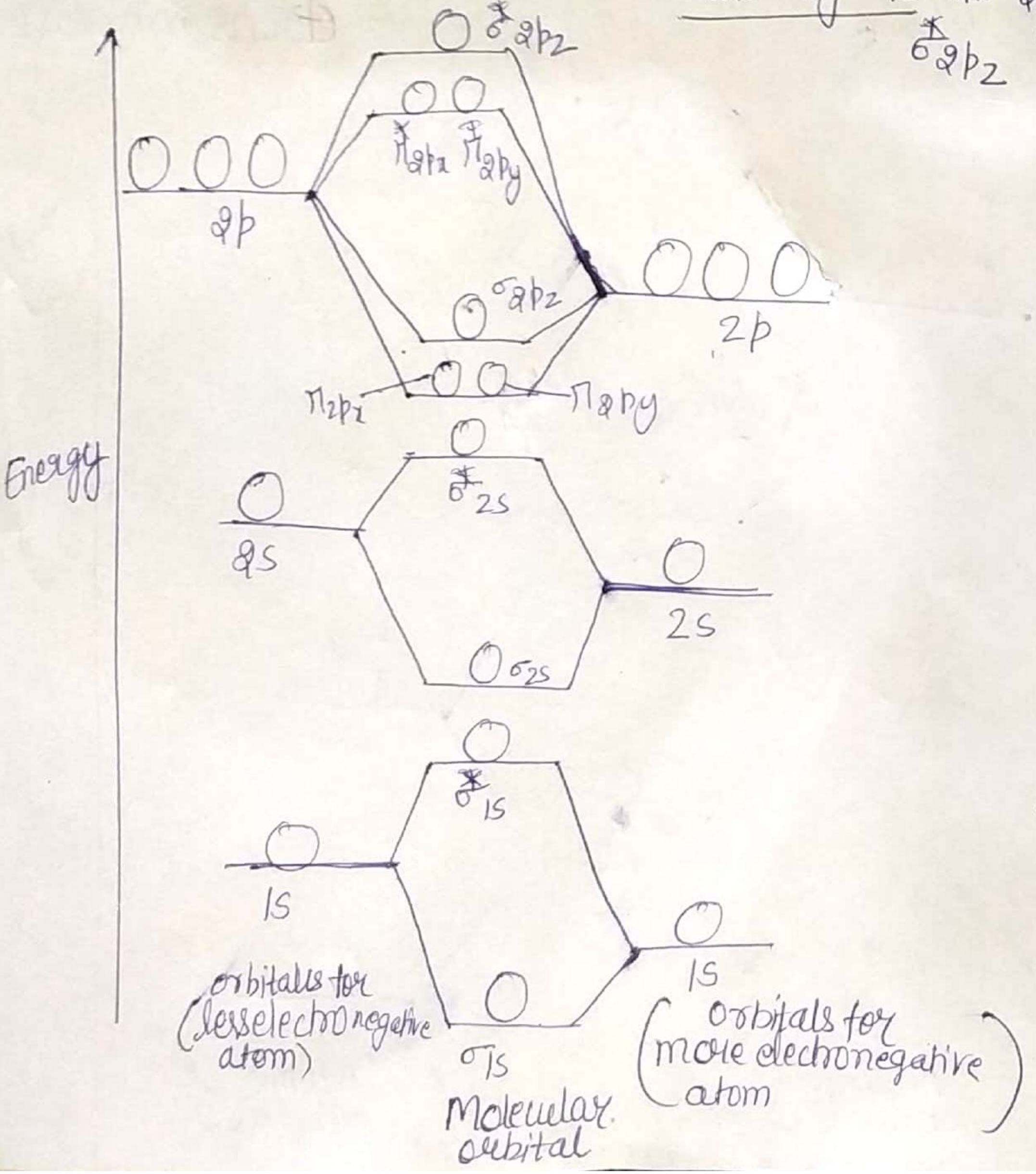


Energy level diagram or Molecular orbital diagram of Heteronuclear diatomic molecules

1. (13e) CN, CO → (14e⁻)

$\downarrow$ CN⁻ $\downarrow$ CO⁺ → upto 14e⁻ increasing order of energy

$\sigma_{1s}\ \overset{*}{\sigma}_{1s}\ \sigma_{2s}\ \overset{*}{\sigma}_{2s}\ \pi_{2p_x}=\pi_{2p_y}\ \sigma_{2p_z}\ \overset{*}{\pi}_{2p_x}=\overset{*}{\pi}_{2p_y}\ \overset{*}{\sigma}_{2p_z}$



1. NO (15e) → NO⁺, NO⁻ → for more than 14e⁻ increasing order of energy

$\sigma_{1s}\ \overset{*}{\sigma}_{1s}\ \sigma_{2s}\ \overset{*}{\sigma}_{2s}\ \sigma_{2p_z}\ \pi_{2p_x}=\pi_{2p_y}\ \overset{*}{\pi}_{2p_x}=\overset{*}{\pi}_{2p_y}\ \overset{*}{\sigma}_{2p_z}$