

Chemical Bonding And Molecular Structure

The force which binds atoms together to form a molecule is called chemical bond and the process of formation of a chemical bond is called chemical bonding.

Atoms possess higher energy in free state. During the formation of a bond, energy is released which results in the decrease of potential energy and the obtained molecule is more stable in comparison to its constituent atoms.

Octet rule → An atom will become ~~stab~~ stable after having eight electrons in its outermost shell because it gain the stability of noble gases. To have eight electrons in its valence shell is called octet rule except helium (2 electron).

The number of electrons an atom of an element loses or gains or shares to attain eight electrons in its ~~outermost~~ shell is called valency of the element.

Outermost shell of an atom is called valence shell and electrons present in it are called valence electrons.

Ionic or Electrovalent Bond

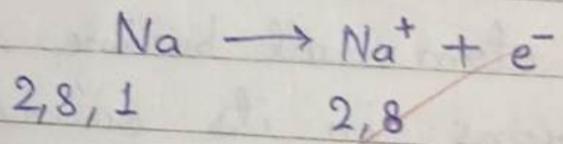
The electrostatic force of attraction which binds cations and anions together is called ionic or electrovalent bond.

There are two type of electrovalent bond:

- 1) Losing electrons
- 2) Gaining electrons

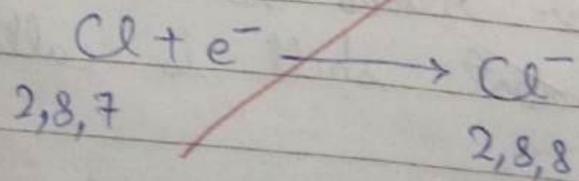
① Losing electrons → In this process, atoms lose valence electrons to form cations. If it is easier to lose some electrons than gain more electron, then atom will lose.

For example →



② Gaining electrons → In this process, atoms take electrons in their valence shell to form anions. If it is easier to gain some electrons than lose more electron, then atom will gain or take.

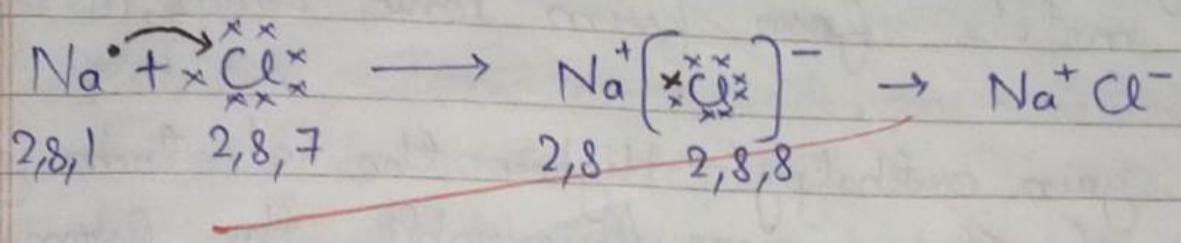
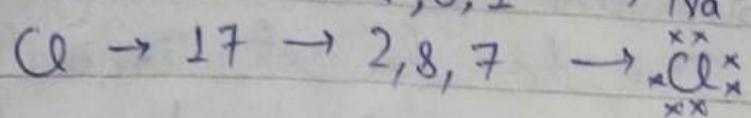
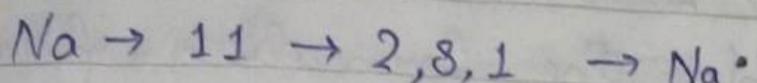
For example →



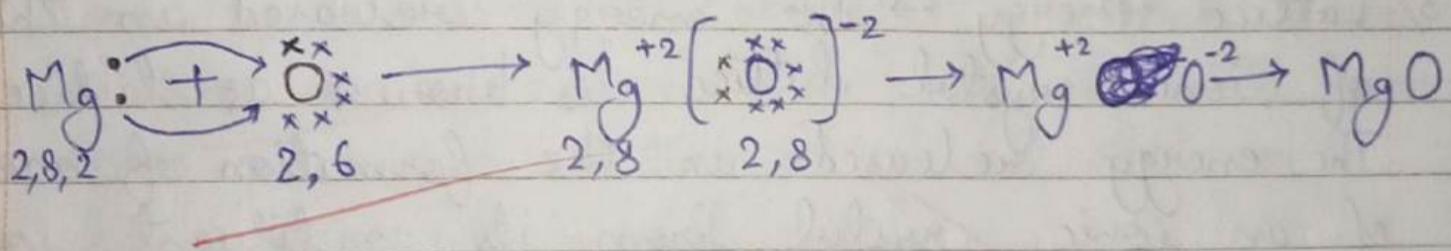
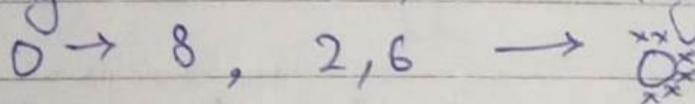
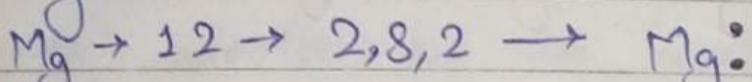
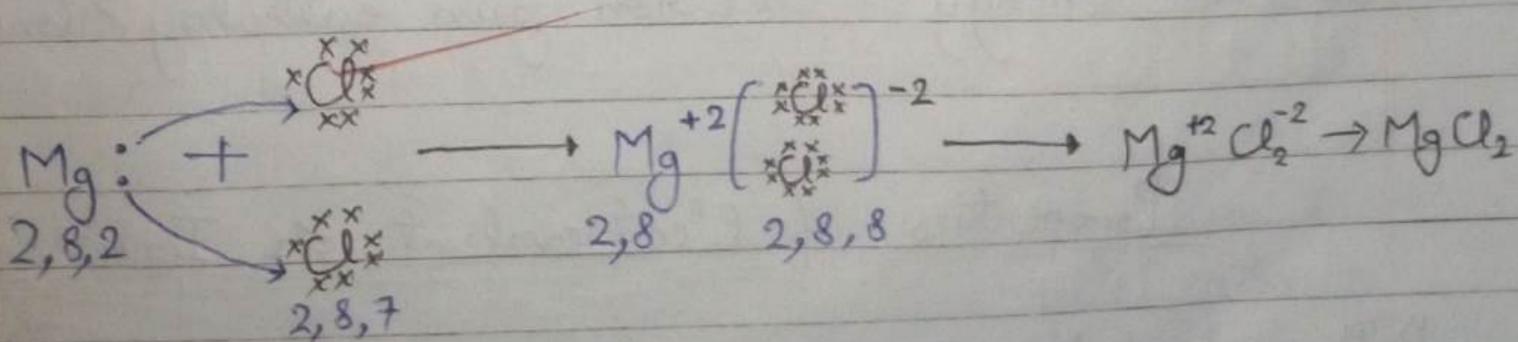
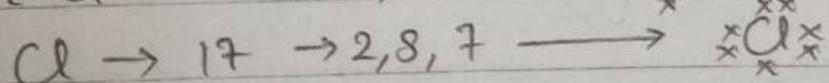
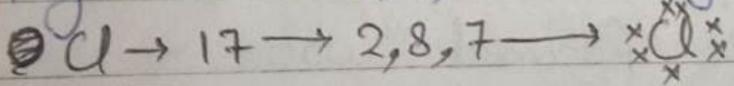
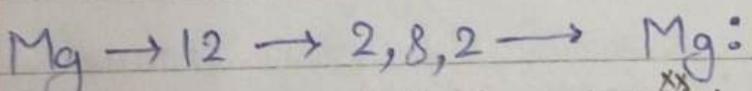
Formation of Ionic Bond

Ex →

① NaCl



② MgO

③ MgCl₂

Factors Influencing Ionic Bond Formation

- 1) Ionization enthalpy → Lower the ionisation energy of atom, more favourable the formation of an ionic bond by the atom. Due to lowest ionisation energy, alkali metals form ionic bonds, most easily.
 - 2) Electron gain enthalpy → Higher the electron gain enthalpy of atom, more favourable the formation of an ionic bond by the atom. Due to maximum electron gain enthalpy, halogens form ionic bonds, most easily.
 - 3) Lattice energy → The energy released in the formation of ionic crystal lattice is known as lattice energy. The energy released in the formation of one mole of an ionic crystal from its constituent ions is called lattice energy of an ionic bond.
Higher the lattice energy, more stable is the ionic bond or ionic compound.
- * Stable ionic bond is formed when

~~lattice energy + electron gain enthalpy > ionization enthalpy~~

Properties of Electrovalent or Ionic Compounds

- 1) Physical state → Ionic compounds exist in crystalline form in solid state.

- 2) Melting and boiling points → A strong electrostatic force of attraction exist among the ions of ionic compounds. Due to this strong electrostatic attractive force these compounds have high melting points and boiling points.
- 3) Solubility → Ionic compounds are soluble in polar solvents like water etc. They are insoluble in non-polar solvents like benzene, carbon tetrachloride etc.
- 4) Electrical conductivity → They are good conductor of electricity in water or molten state.
- 5) Ionic reactions → No chemical reactions occurs between ionic compounds in solid state. This process takes place in solution or fused state only.

Covalent Bond

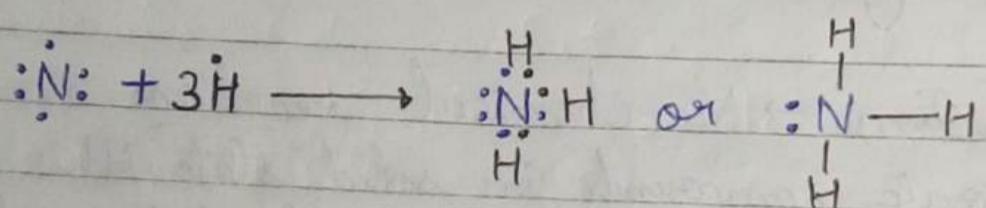
The bond formed between two atoms by mutual sharing of electrons is called covalent bond. The compound thus formed is called covalent compound.

The following rules are followed in the formation of this bond:

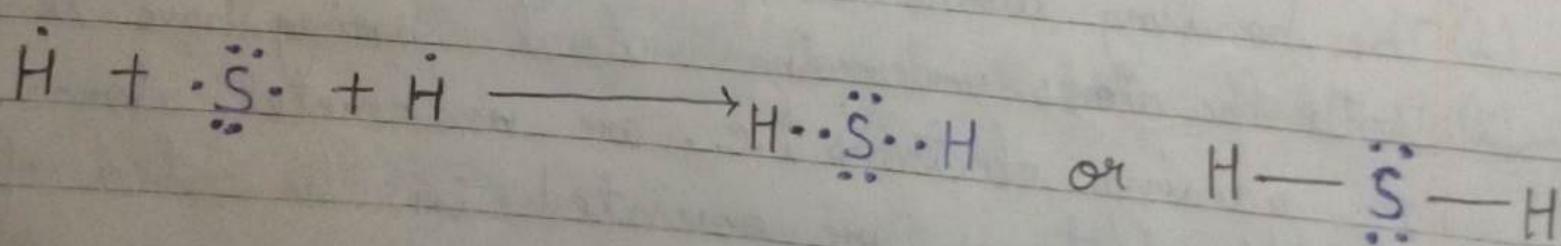
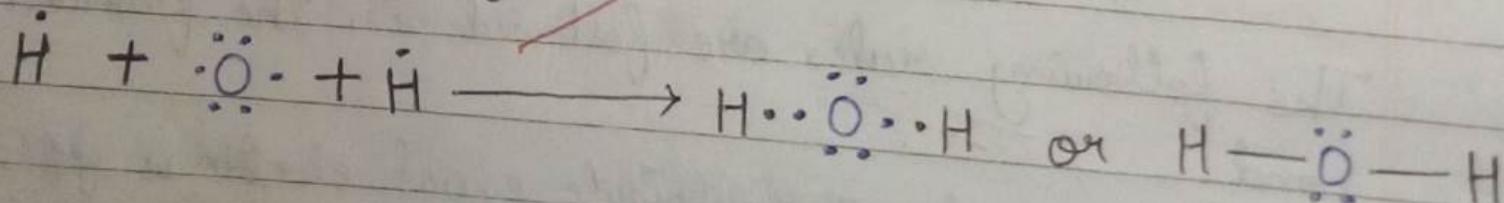
- (1) The bonding atoms contribute equal electrons for sharing.
- (2) Both the atoms undergoing mutual sharing have tendency of gaining electrons i.e., are non-metal atoms.
- (3) Shared electrons are counted in the octet of both the atoms.

Examples →

(a) Formation of molecule of ammonia → Outermost shell of atom of nitrogen contains 5 electrons. Hence, it needs only three electrons to attain a stable state. Atom of hydrogen needs only one more electron to attain helium gas configuration. Therefore nitrogen atom shares three electrons, one each, with three hydrogen atoms. As a result, eight electrons are acquired by the outermost shell of nitrogen and two electrons by first shell of each hydrogen atom to form a stable compound.

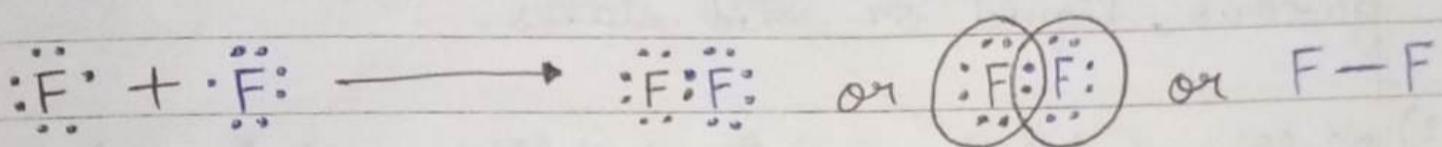


(b) Formation of water and hydrogen sulphide → Both these molecules are formed by a covalent bond. In the outermost shell of atoms of both oxygen and sulphur there are 6 electrons. Their octets are completed by two atoms of hydrogen. Sharing between atoms of hydrogen and atoms of these elements occurs in the following way:

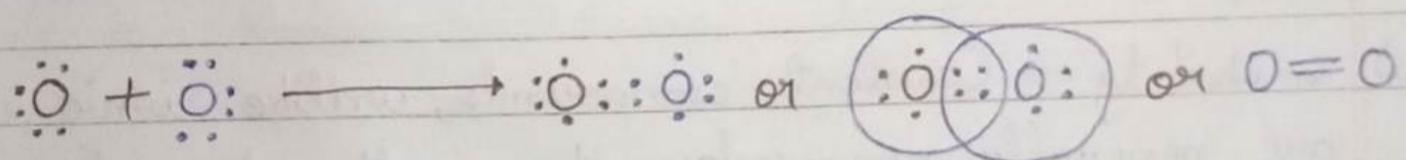


Covalent bonds are of three types :

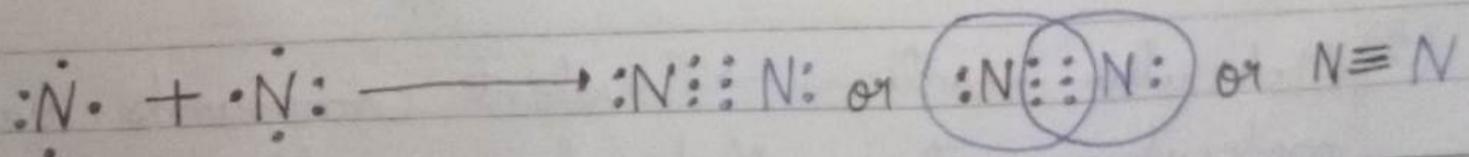
(1) Single covalent bond — This bond is formed by the mutual sharing of two electrons between two atoms. Each atom contributes one electron for sharing. This bond is represented by a small line (-) between the atoms. Like F_2 molecule —



(2) Double covalent bond — This covalent bond is formed between two atoms by the mutual sharing of four electrons. Each atom contributes two electrons for sharing. This bond is denoted by two small horizontal lines (=) between the two atoms. Like O_2 molecule —



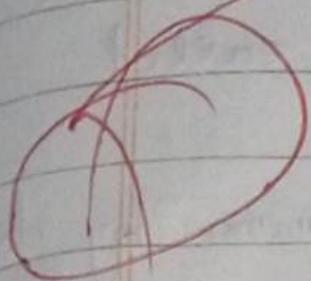
(3) Triple covalent bond — This covalent bond is formed between two atoms by the mutual sharing of six electrons. Each atom gives three electrons for sharing. This bond is denoted by three small horizontal lines (\equiv) between the two atoms. Like, nitrogen molecule.



Properties of Covalent Compounds

- (1) Physical state → In the molecules of covalent compounds, atoms are bonded with each other through mutual sharing of electrons. Weak vander Waal's forces exist between the covalent compound molecules. Due to this, covalent compounds exist in gaseous, liquid or solid states.
- (2) Melting and boiling points → Melting points and boiling points of covalent compounds are lower than ionic compounds due to weak vander Waal's forces between molecules. Only covalent compounds with giant molecules like diamond, silicon carbide etc. have high melting points and boiling points.
- (3) Solubility → Covalent compounds, unlike ionic compounds, are generally non-polar. Hence, they do not dissolve in polar solvents like water etc., but are soluble in non-polar solvents like benzene, carbon tetra-chloride etc.
- (4) Electrical conductivity → Covalent compounds do not form ions in fused state or in solution. Hence, they are bad conductors of electricity.
- (5) Molecular reactions → Covalent compounds undergo molecular reactions. Molecular reactions are slower in comparison to ionic reactions. These reactions require catalysts, pressure and heat to occur.

(6) Isomerism \rightarrow Covalent bonds are directional, due to which these compounds exhibit isomerism.



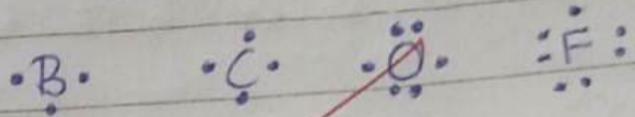
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Lewis Structure

The symbols used by G.N. Lewis to represent valence electrons in an atom are called Lewis symbols.

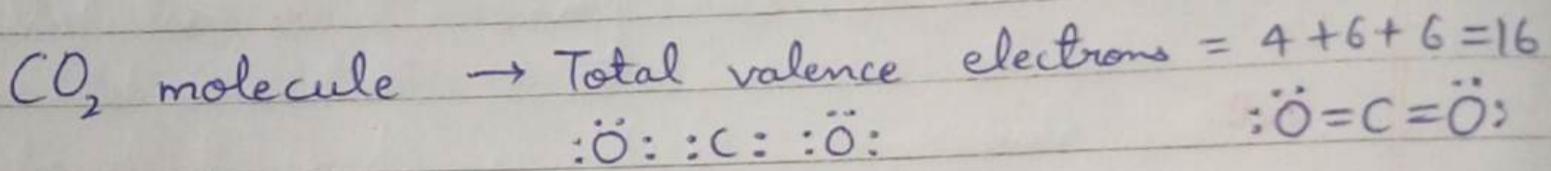
Electrons of outermost shell are shown by dots around the symbol of elements.

Like -



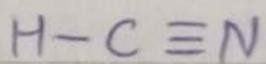
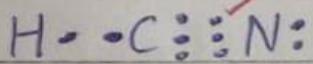
~~The molecular structure represented by Lewis symbols is called Lewis structure.~~

Ex → ~~:N::N:~~



HCN molecule →

$$\text{Total valence electrons} = 1+4+5=10$$



Bond Parameters

These characteristic constants of a covalent bond e.g., bond energy, bond length and bond angle are called bond parameters.

Bond Energy or Bond Enthalpy

The minimum energy required to break one mole bond in the gaseous state of a substance, is called its bond energy.

- ① Atomic size → The larger the size of bonding atoms the more is distance between them, hence lower will be the bond energy.
- ② Multiplicity of bonds → The existence of more than one bond between two atoms is called multiplicity of bond. Greater the number of bonds between atoms shorter is the distance between them.

Bond Length

The bond length of a bond is the distance between the nuclei of the bond forming atoms.

- ① Atomic size → Nuclei of bond forming atoms are at a large distance if the atomic size is large. Thus, larger the atomic size more lengthy is the bond.
- ② Multiplicity of bonds → Bond length decreases when there is more than one bond between the bonding -

atoms. Hence, greater the number of bonds between the bond forming atoms, shorter is the bond length.

Bond Angle

When two atoms separately form bond with third atom, then two bonds are formed. The angle between these two bonds is called bond angle.

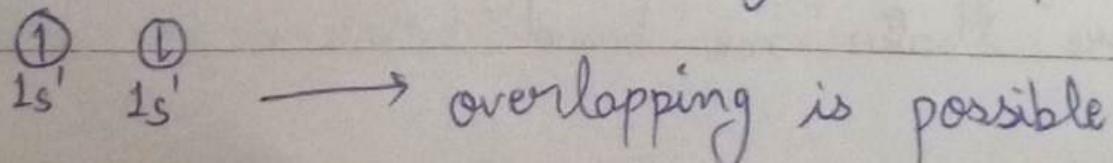
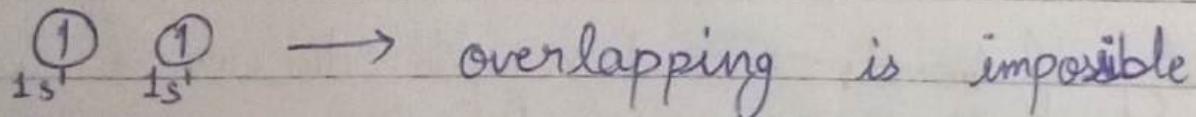
Bond Order

Number of bonds between two atoms of a molecule is called bond order.

Valence Bond Theory

Valence Bond Theory was proposed in 1927 by Heitler and London.

- ① Covalent bond formation is possible between two atoms which have at least one unpaired electron in an orbital of their valence shell.
- ② For the bond formation between two atoms, the nuclei of each atom attracts the orbital having unpaired electron of the other atom.
- ③ This attraction ~~and~~ results into the overlapping of orbitals having unpaired electrons of bond forming atom.
- ④ The overlapping reduce energy and is responsible for covalent bond
- ⑤ This overlapping take place between the orbital having unpaired electrons with the opposite spin.



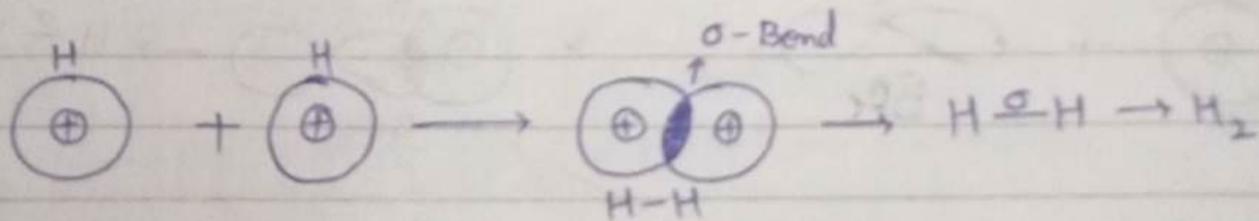
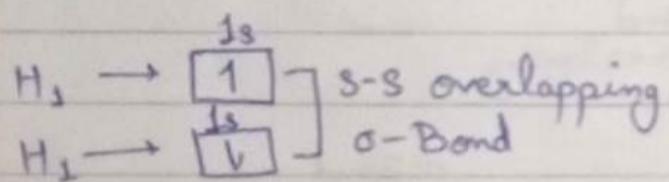
Overlapping of Atomic Orbitals

When two atoms come close to each other to form bond, their overlapping may be positive, negative or zero.

Types of Overlapping

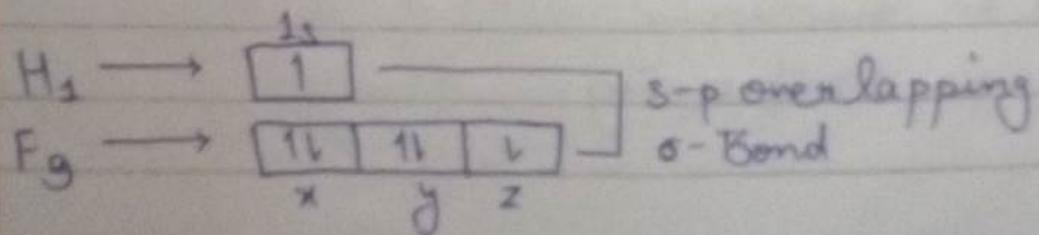
- ① s-s overlapping → This overlapping takes place between two s-orbitals. These s-orbitals have one-one unpaired electron with opposite spin. It is also called coaxial overlapping. The bond so formed is called the ^{sigma} (σ) bond.

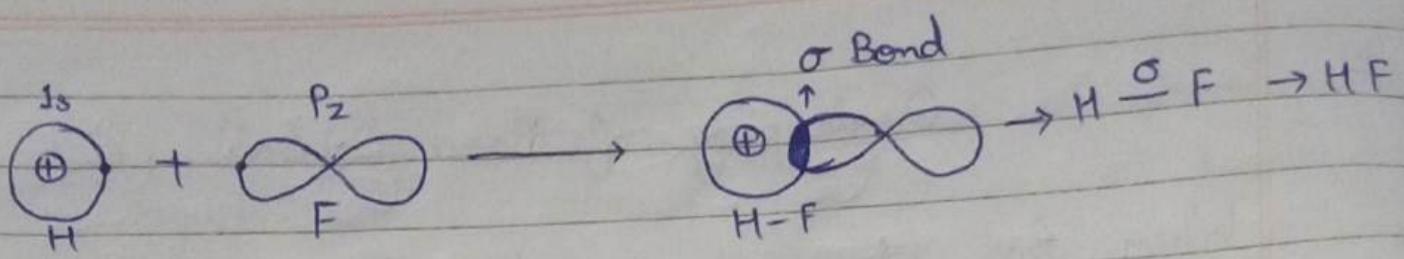
Ex → Formation of H_2 molecule



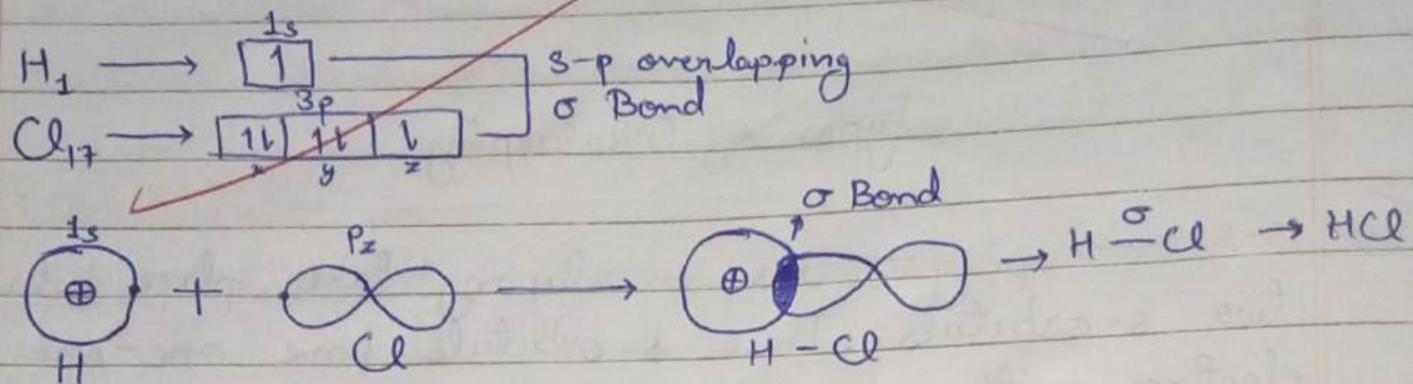
- ② s-p overlapping → This overlapping takes place between one s- and one p-orbital. The s- and p-orbitals involved in overlapping have one electron each with opposite spin.

Ex → Formation of HF molecule

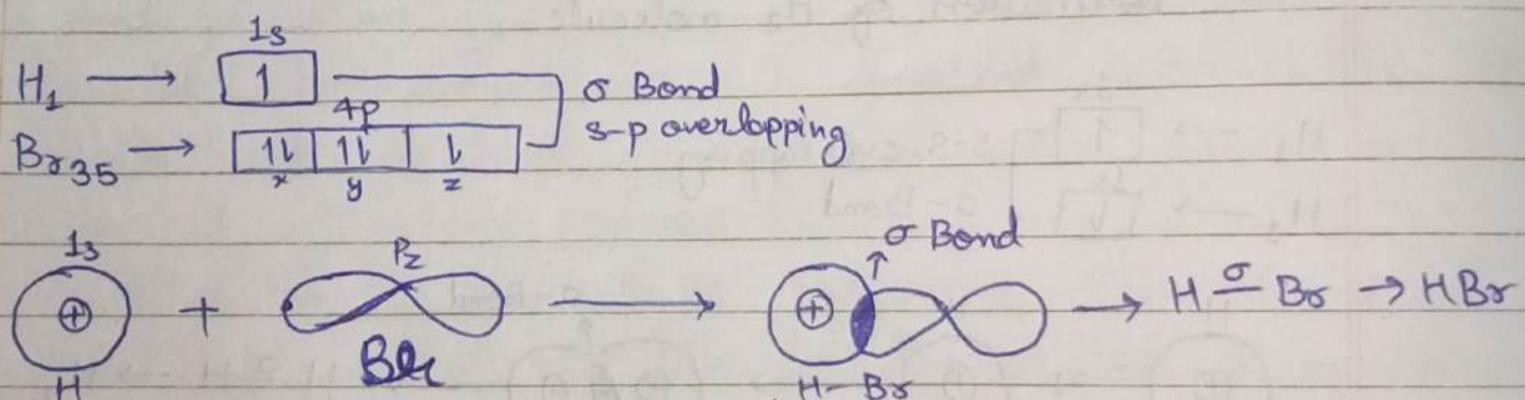




Formation of HCl



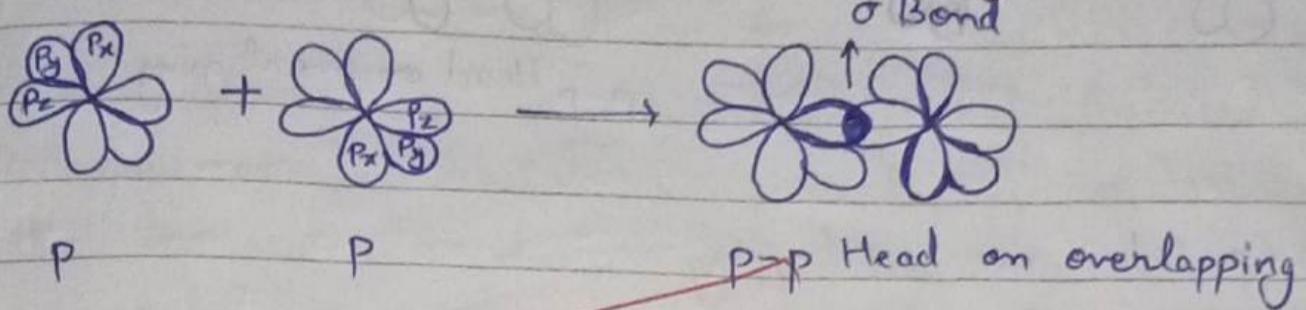
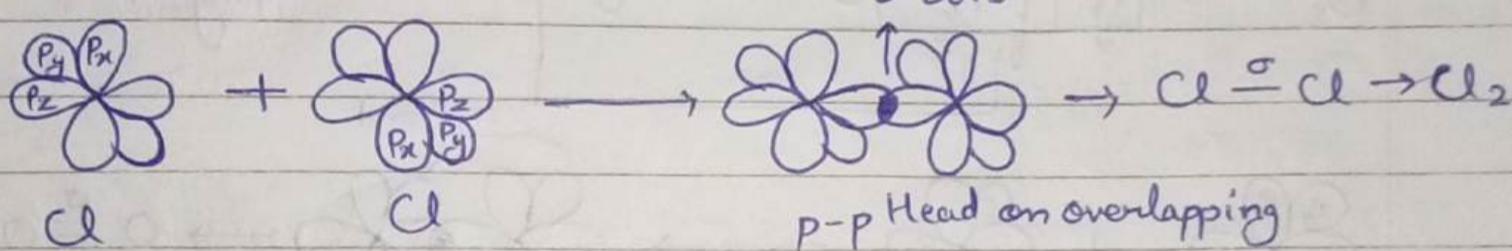
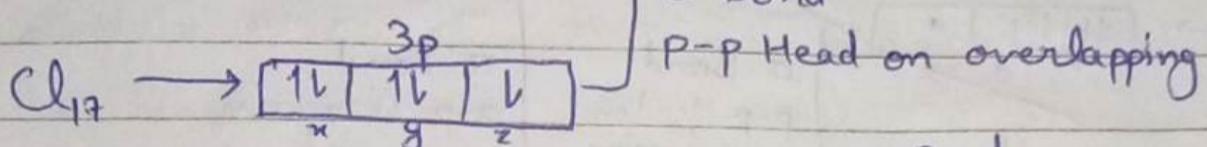
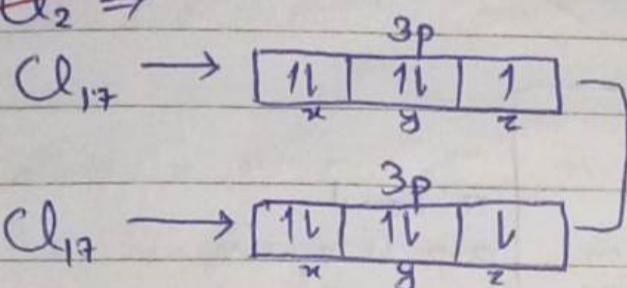
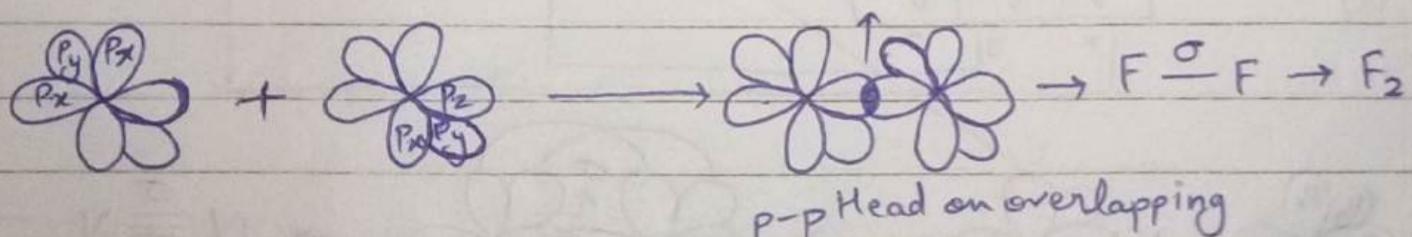
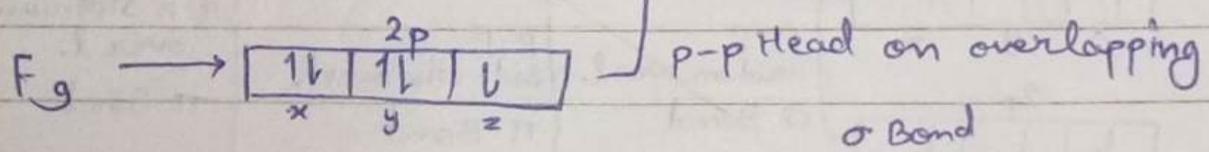
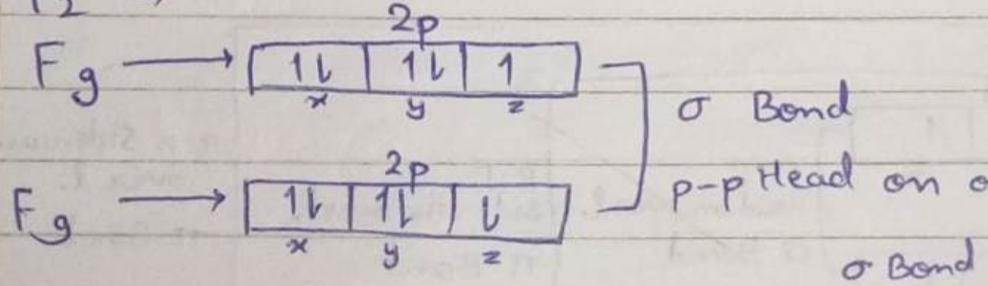
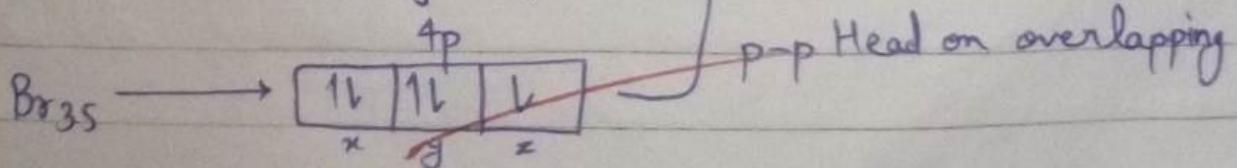
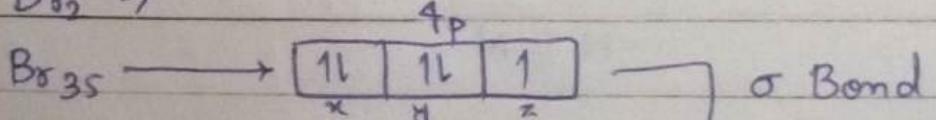
Formation of HBr

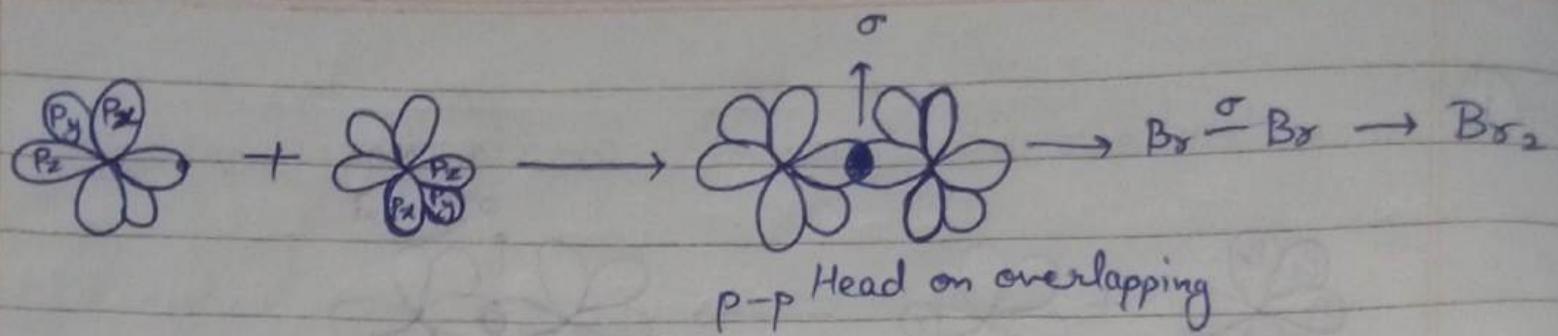


③ ~~p-p overlapping~~ → This overlapping takes place between two p - orbitals . It is necessary that both the p - orbitals have one electron each with opposite spin . p - orbitals are directed towards three x, y and z - axes.

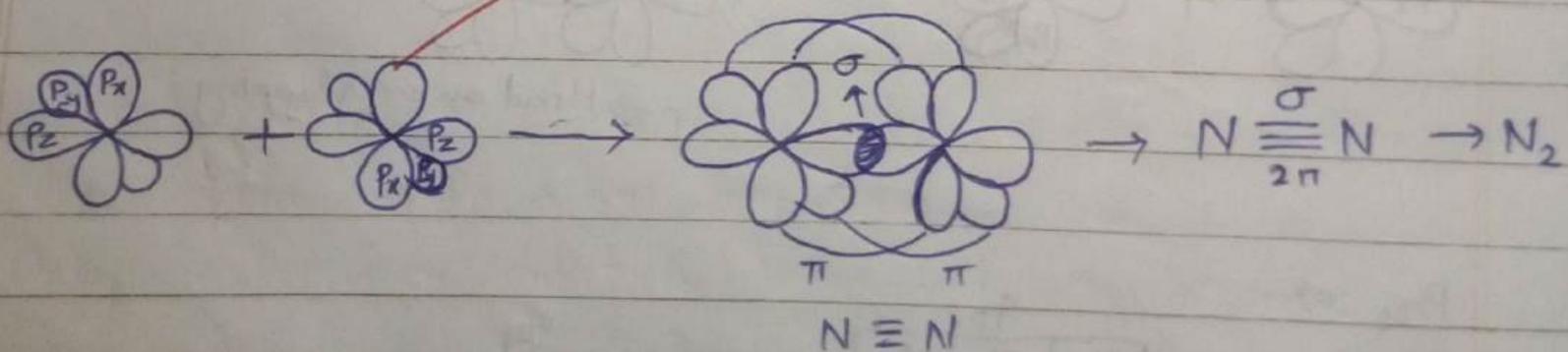
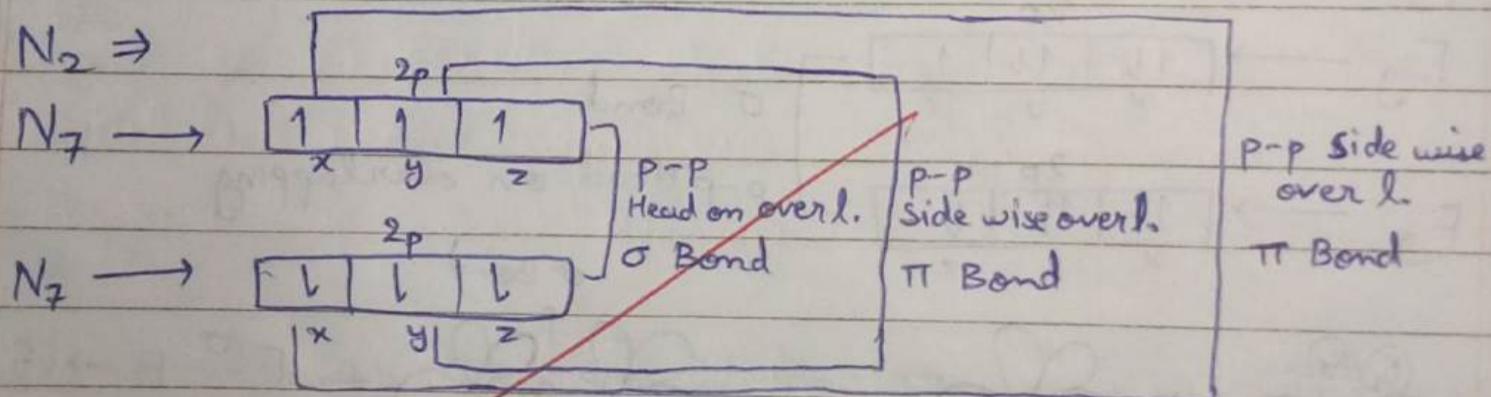
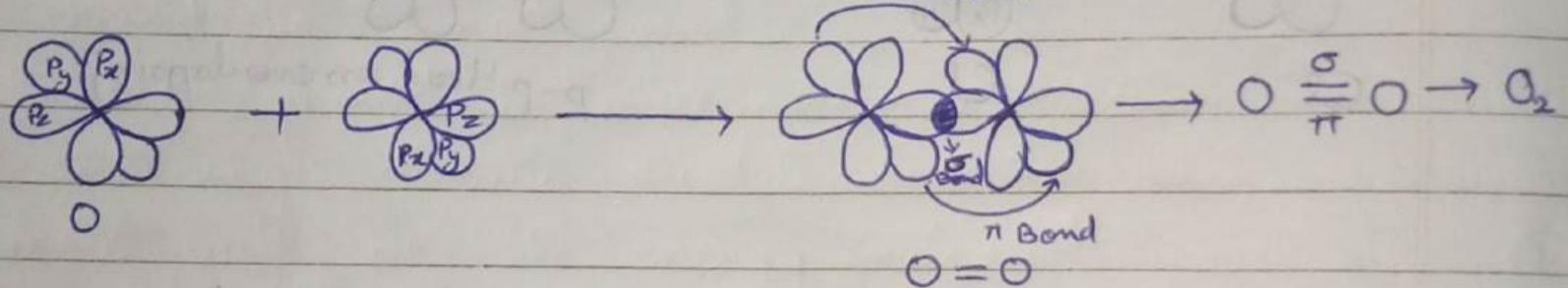
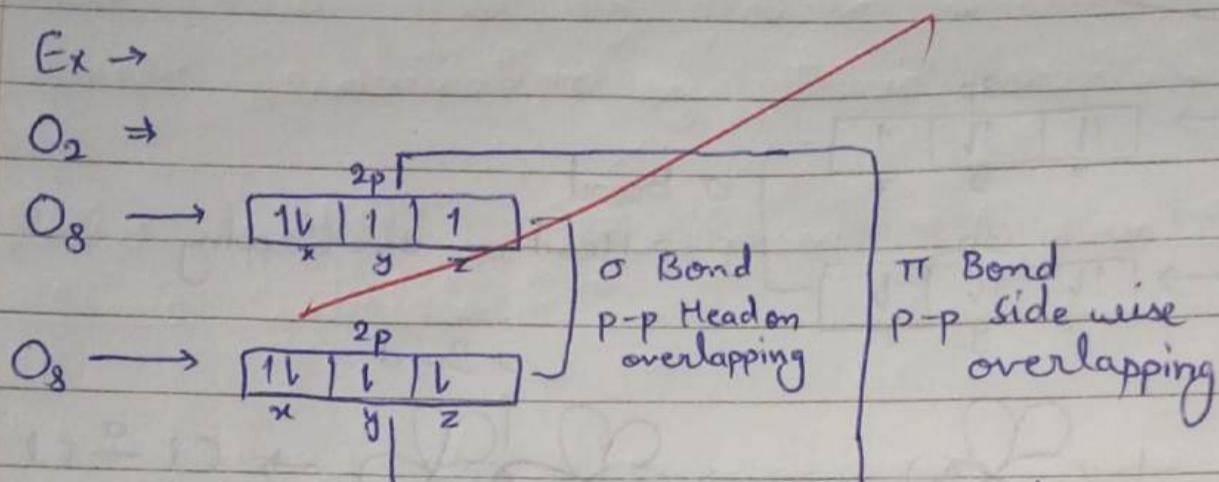
- i) p - p Head on overlapping
- ii) p - p side wise overlapping

i) p-p Head on OR coaxial overlapping :-

 $E_x \rightarrow$ ~~$\text{Cl}_2 \Rightarrow$~~  $F_2 \Rightarrow$  $\text{Br}_{35} \Rightarrow$ 



ii) $p-p$ Side wise overlapping

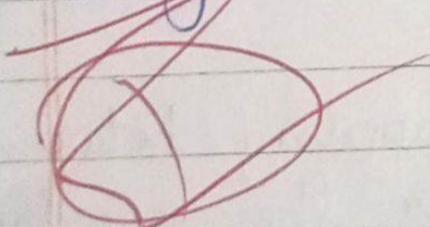


Sigma (σ) Bond

- ① The bond formed by the coaxial overlapping of the orbitals is called the sigma bond.
 - ② This overlapping takes place along the internuclear axis.
 - ③ This bond is comparatively stronger.
 - ④ The first overlapping between two atoms forms a sigma bond always.

Pi (π) Bond

- ① A bond formed by lateral overlapping of orbitals is called pi-bond.
 - ② This overlapping takes place between orbitals of parallel axis perpendicular to the internuclear axis.
 - ③ This bond is comparatively weak.
 - ④ This overlapping is possible only after coaxial overlapping.



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Molecular Orbital Theory

In 1932 Hund and Mulliken presented the Molecular Orbital Theory.

According to this theory, to form a molecule from atoms, the atomic orbitals of atoms combine together to form molecular orbitals. This combination of atomic orbitals is called linear combination of atomic orbitals (LCAO).

~~Main Conditions to form Molecular Orbitals from Atomic Orbitals~~

- 1) The energy of the combining atomic orbitals should be almost equal.
- 2) There should be maximum overlapping between the combining atomic orbitals. Greater the overlapping more will be the energy released resulting into greater stability.
- 3) It is necessary that the combining atomic orbitals are symmetric along internuclear axis. Asymmetric overlapping is not possible.

Main Postulates of Molecular Orbital Theory

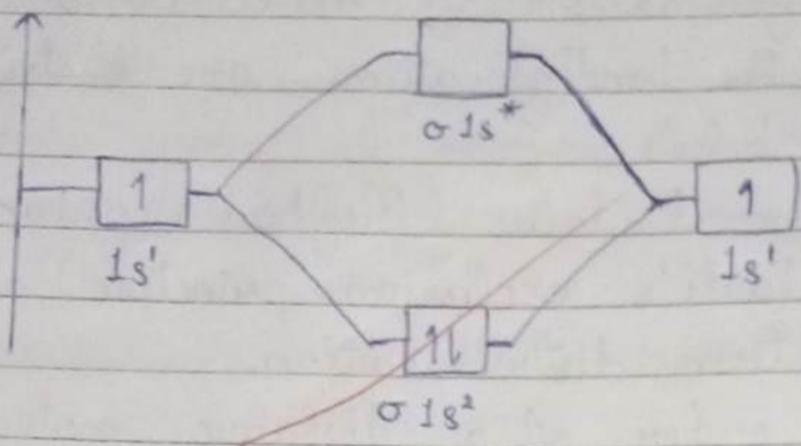
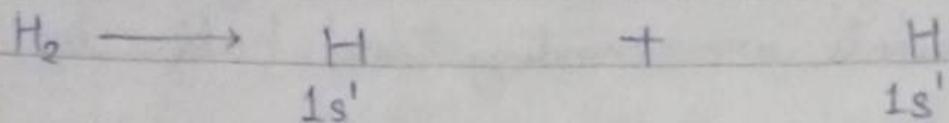
- 1) The atomic orbitals of the bonding atoms combine to form molecular orbitals.
- 2) Only molecular orbitals formed by atomic orbitals of valence shell take part in bond formation. The molecular orbitals formed by other atomic orbitals are non-bonding molecular orbitals.

- 3) The number of molecular orbitals obtained is equal to the number of atomic orbitals. Half of the molecular orbitals are bonding and half are antibonding.
- 4) After the formation of molecular orbitals the electrons of the bonding atoms are distributed in molecular orbitals.
- 5) All the general laws (Aufbau's principle, Hund's rule and Pauli's exclusion principle) are obeyed during electron distribution.
- 6) The bond order of a diatomic molecule is determined by the following formula:

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

- 7) Higher the bond order, lower is the bond length and higher is the bond strength.
- 8) The bond order of isoelectronic molecules or ions is equal.

1) Structure of hydrogen molecule —

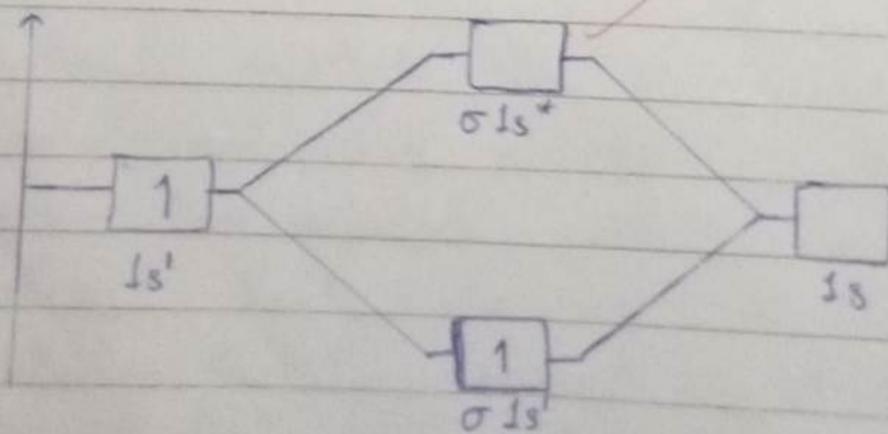
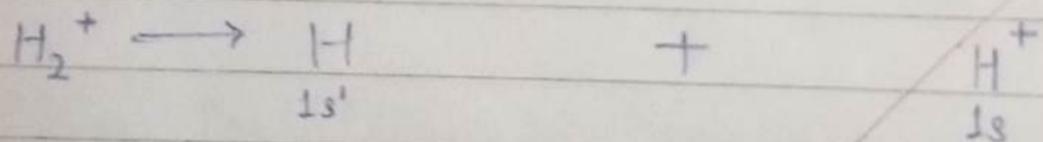


Structure of hydrogen molecule cation (H_2^+) —

$$\text{Bond order} = \frac{N_b - N_a}{2} \Rightarrow \frac{1-0}{2} \Rightarrow 1 \quad [\text{H}-\text{H}]$$

Magnetic property \Rightarrow Due to presence of e^\ominus paired form in M.O. of H_2 . So, it is di magnetic in nature.

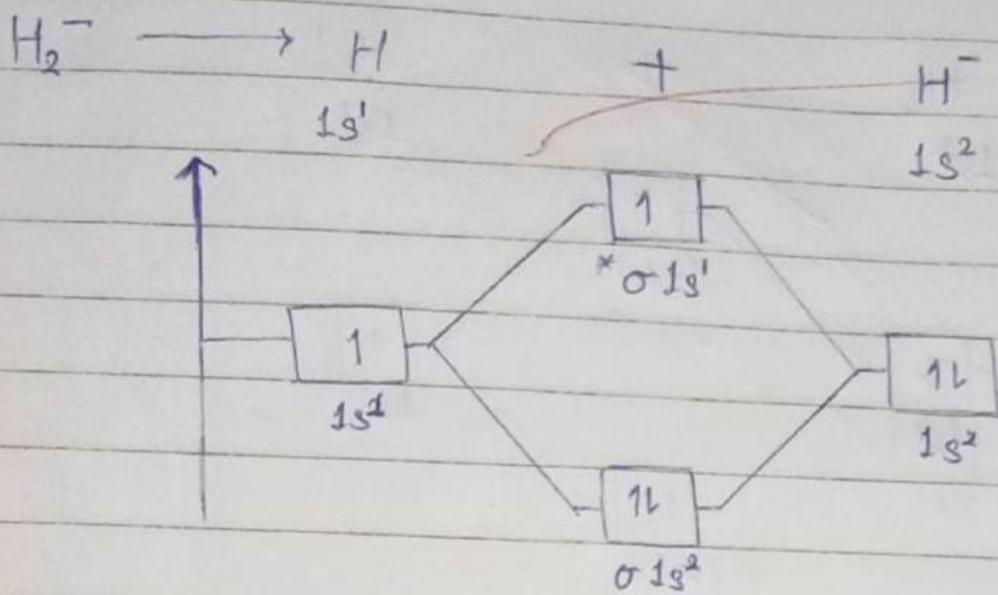
(*) Structure of hydrogen molecule cation (H_2^+) —



$$\text{Bond order} = \frac{N_b - N_a}{2} \Rightarrow \frac{1-0}{2} \Rightarrow 0.5$$

Magnetic property \Rightarrow Due to presence of e[⊖] unpaired form in M.O. of H₂⁺. So it is paramagnetic in nature.

- ① Structure of hydrogen molecule anion (H₂⁻) —

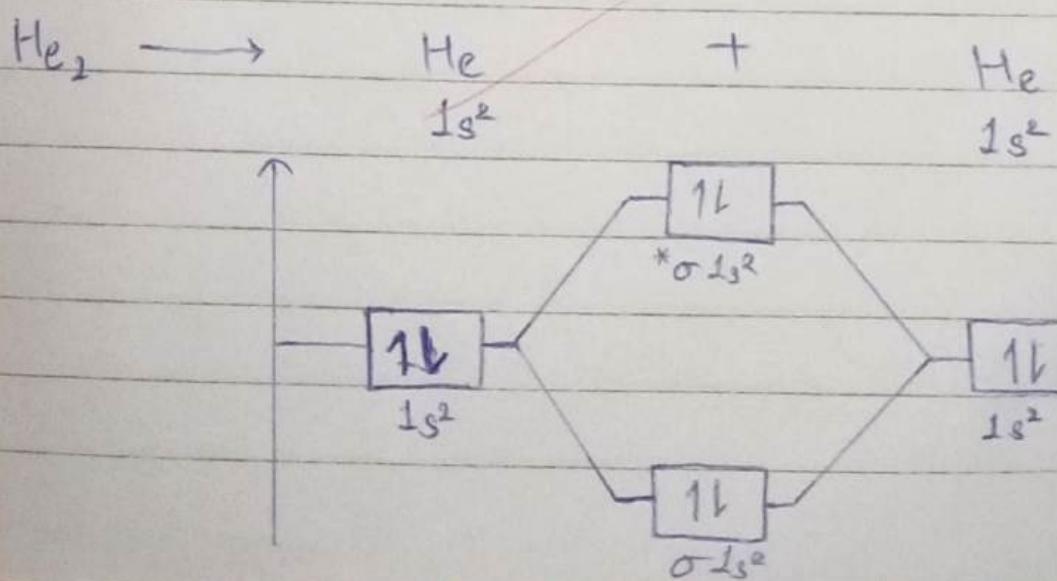


- 2) Structure of heli

$$\text{Bond order} = \frac{N_b - N_a}{2} \Rightarrow \frac{2-1}{2} \Rightarrow 0.5$$

Magnetic property \Rightarrow Due to presence of e[⊖] unpaired form in M.O. of H₂⁻. So, it is paramagnetic in nature.

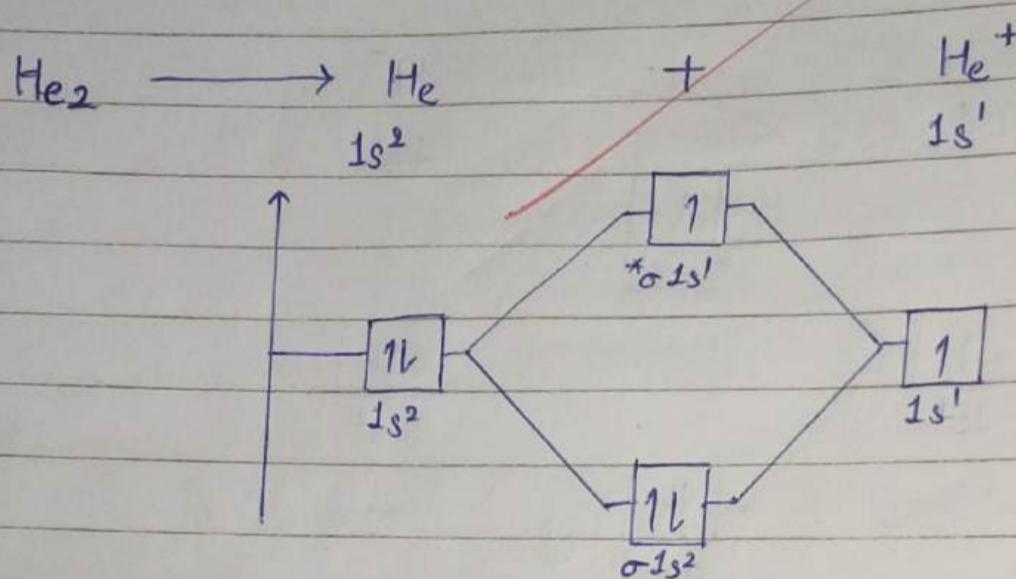
- 2) Structure of helium molecule —



$$\text{Bond order} = \frac{N_b - N_a}{2} \Rightarrow \frac{2-2}{2} \Rightarrow 0$$

Magnetic property \Rightarrow Due to presence of paired e^- in M.O. of He_2 . So it is a Di magnetic in nature.

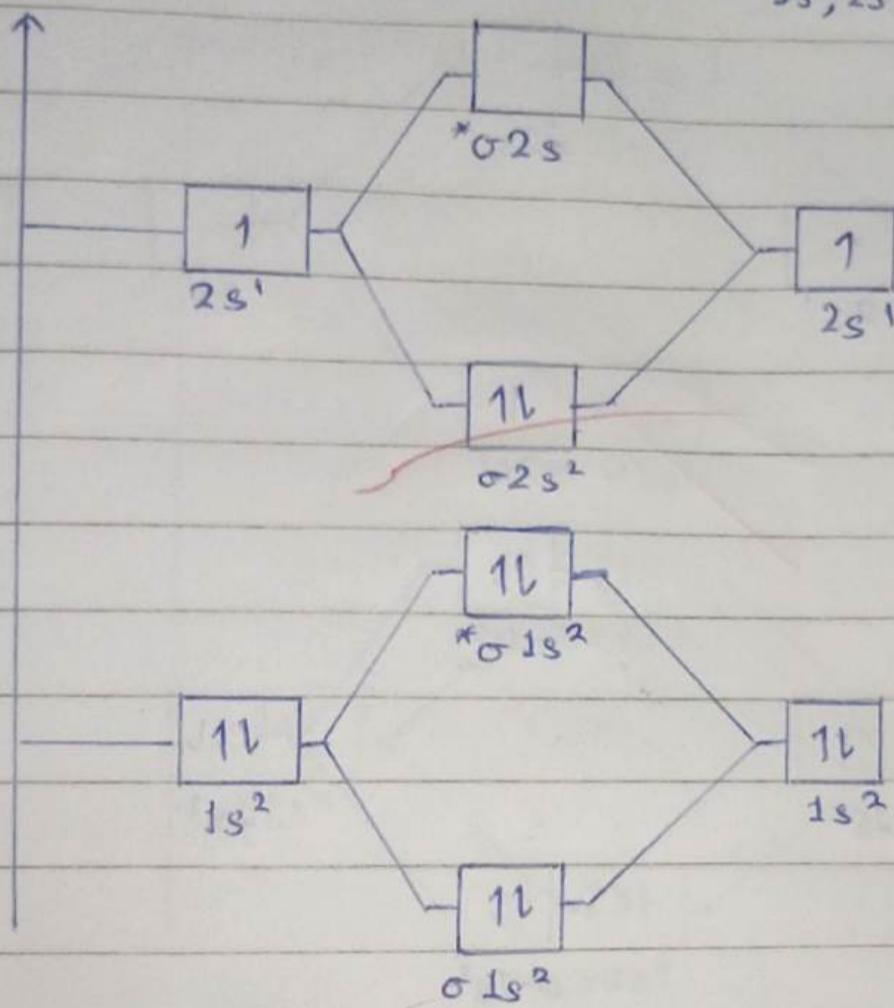
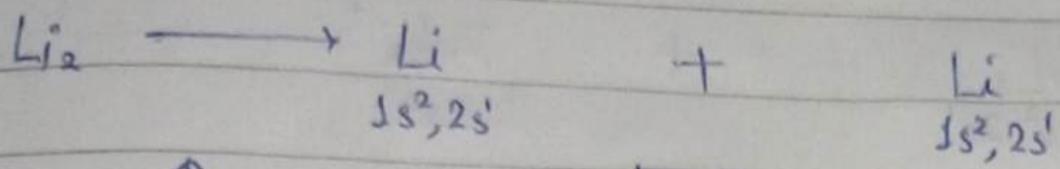
* Structure of Helium molecule cation (He_2^+)



$$\text{Bond order} = \frac{N_b - N_a}{2} \Rightarrow \frac{2-1}{2} \Rightarrow 0.5$$

Magnetic property \Rightarrow Due to presence of unpaired e^- in M.O. of He_2^+ . So it is a para magnetic in nature.

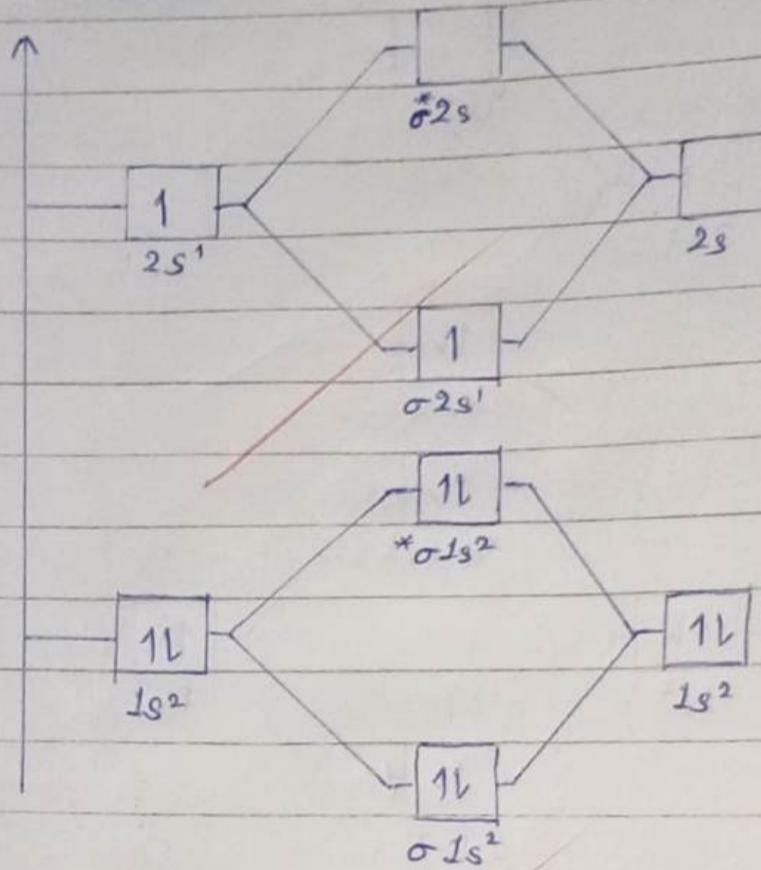
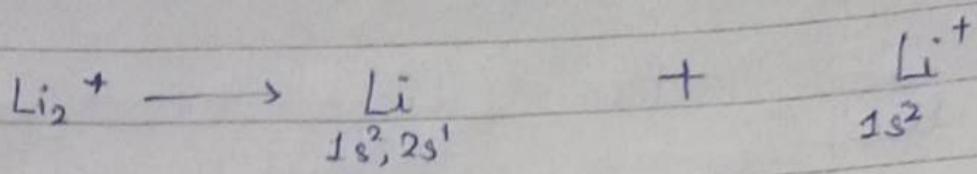
3) Structure of Lithium molecule →



$$\text{Bond order} = \frac{\text{Nb} - \text{Na}}{2} \Rightarrow \frac{4 - 2}{2} \Rightarrow 1 \quad [\text{Li} - \text{Li}]$$

Magnetic property \Rightarrow Due to presence of paired e^- in M.O. of Li_2 .
So it is a Di magnetic in nature.

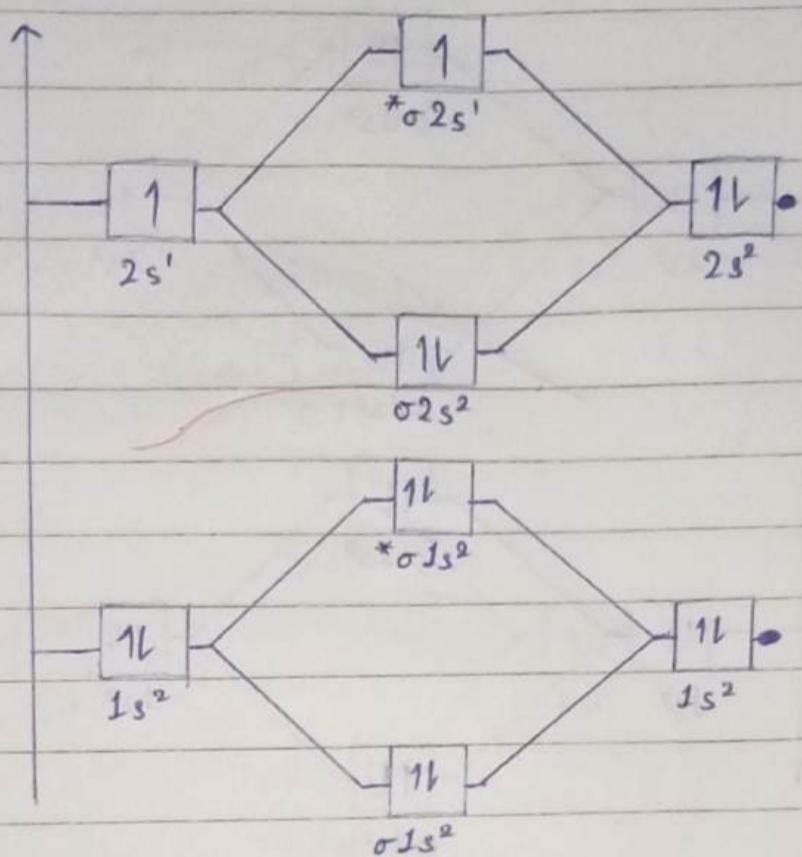
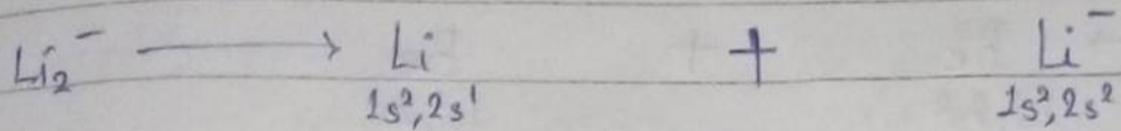
* Structure of Lithium molecule cation (Li_2^+) -



$$\text{Bond order} = \frac{N_b - N_a}{2} \Rightarrow \frac{3-2}{2} = 0.5$$

Magnetic property \Rightarrow Due to presence of unpaired e^- in M.O. of Li_2^+ . So it is a para magnetic in nature.

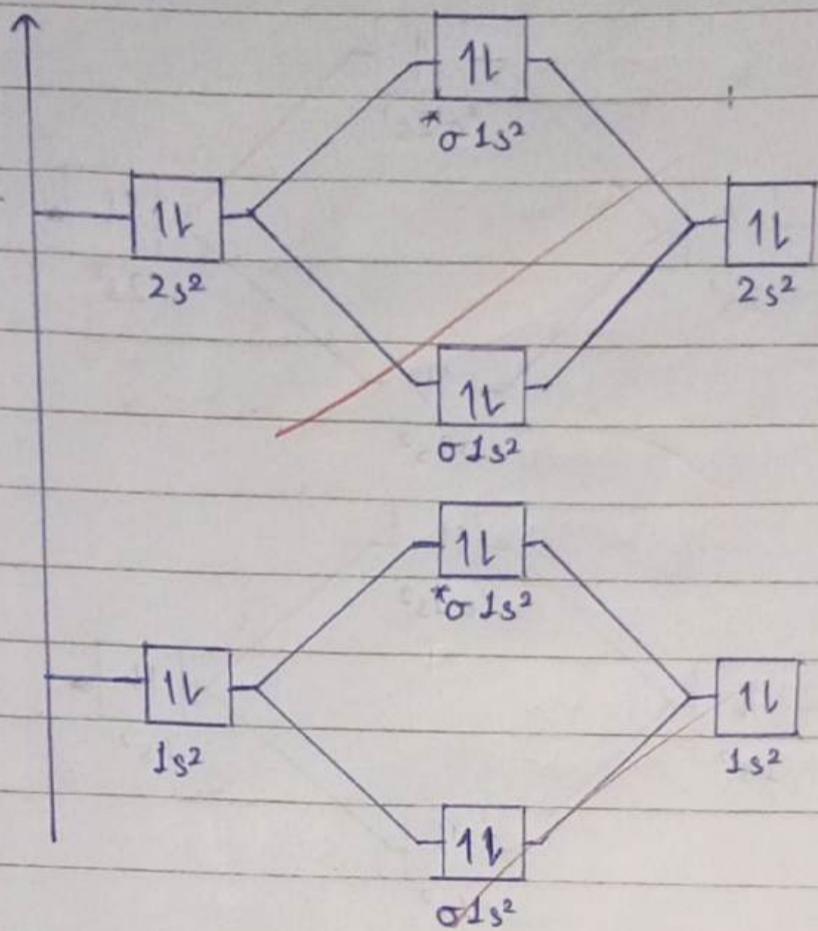
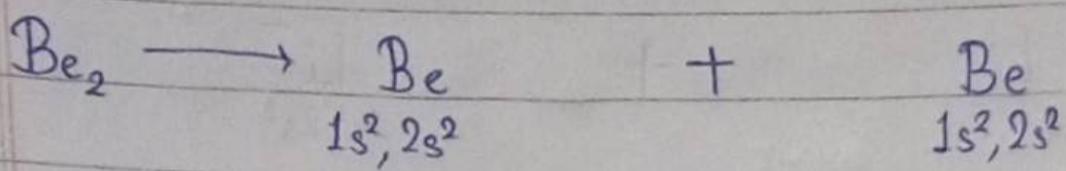
* Structure of Lithium molecule anion (Li_2^-) —



$$\text{Bond order} = \frac{N_b - N_a}{2} \Rightarrow \frac{4 - 3}{2} = 0.5$$

Magnetic property \Rightarrow Due to presence of unpaired e^\ominus in M.O. of Li_2^- . So it is a paramagnetic in nature.

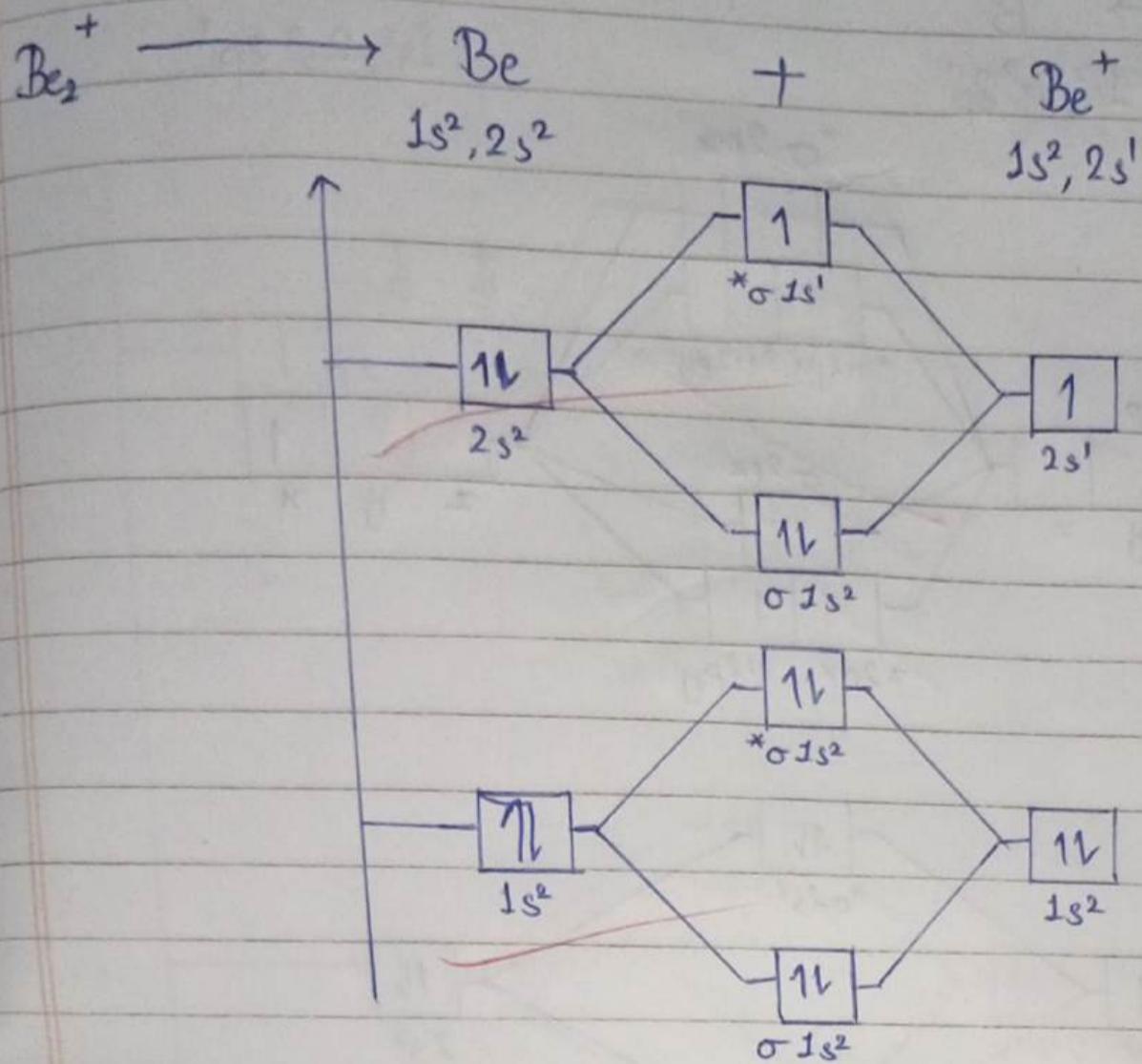
4) Structure of Beryllium molecule -



$$\text{Bond order} = \frac{N_b - N_a}{2} \rightarrow \frac{4 - 4}{2} \rightarrow 0$$

Magnetic property \Rightarrow Due to presence of paired e^- in M.O. of Be_2 . So it is di magnetic in nature.

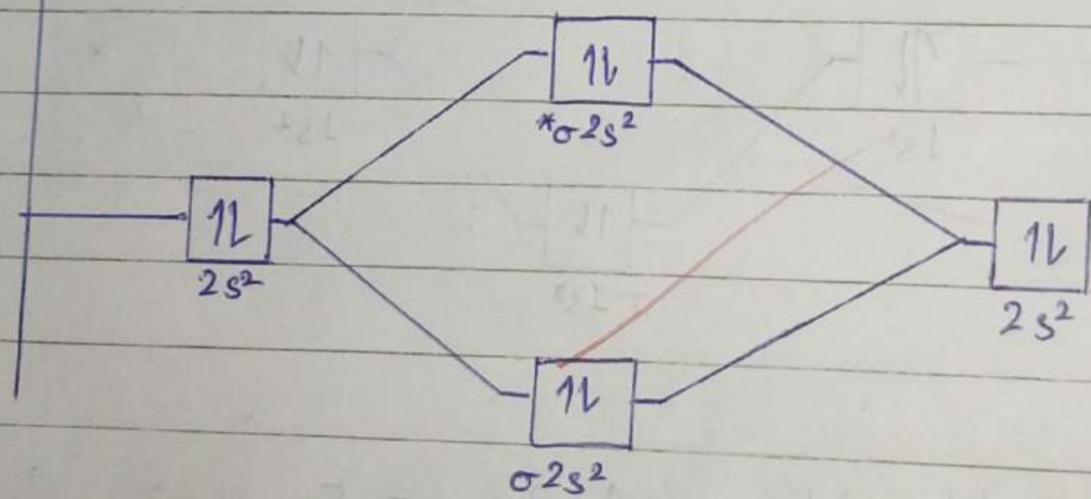
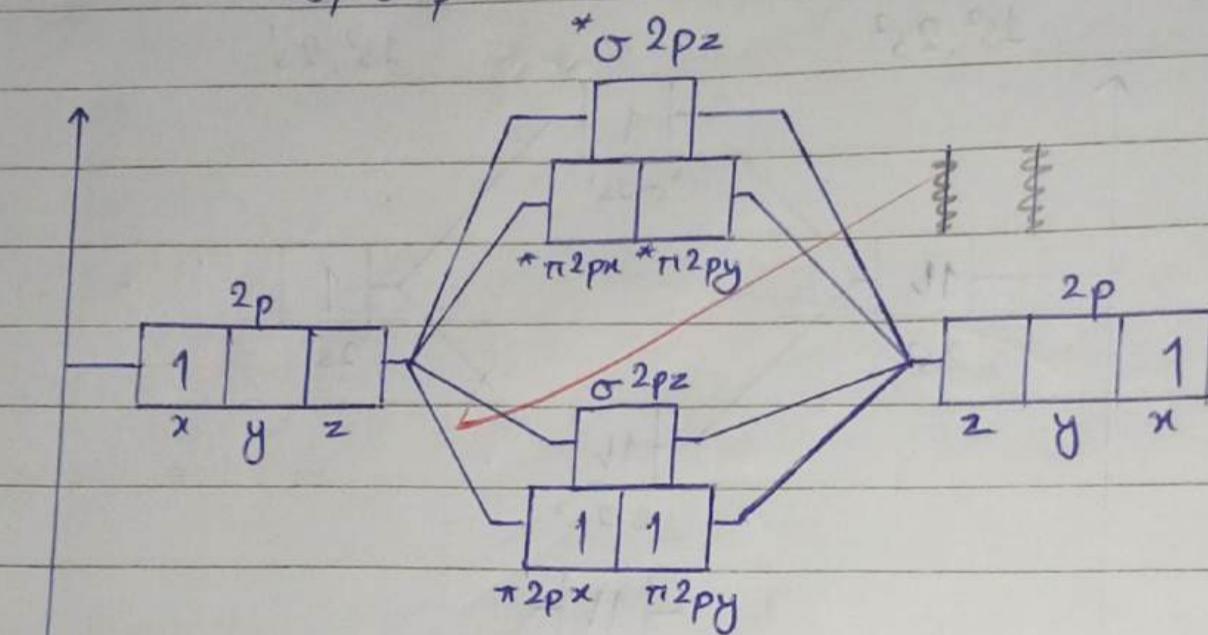
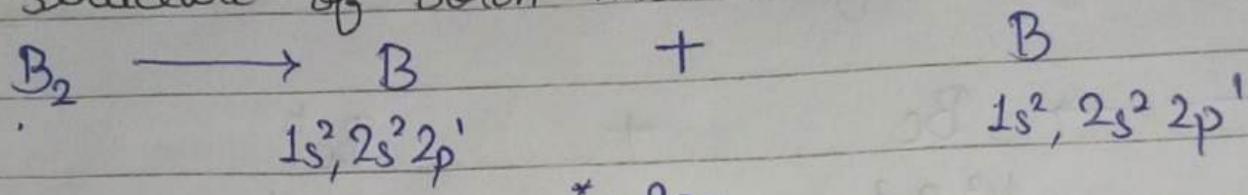
* Structure of Beryllium molecule cation (Be_2^+) -



$$\text{Bond order} = \frac{N_b - N_a}{2} \Rightarrow \frac{4 - 3}{2} \Rightarrow 0.5$$

Magnetic property \Rightarrow Due to presence of unpaired e⁻ in M.O. of Be_2^+ . So it is para magnetic in nature.

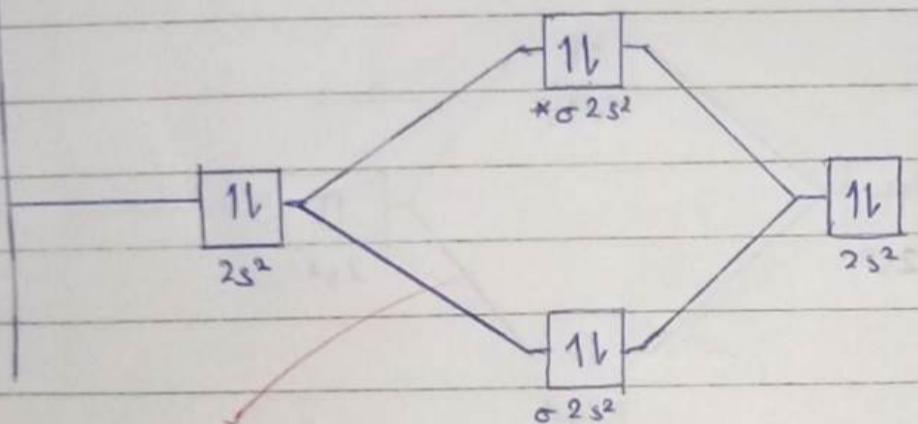
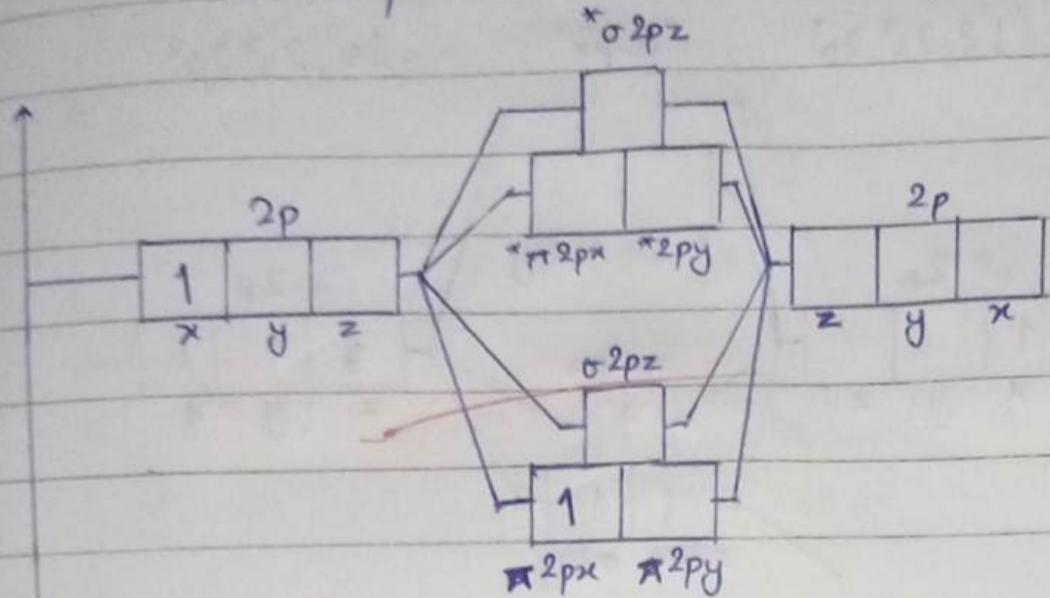
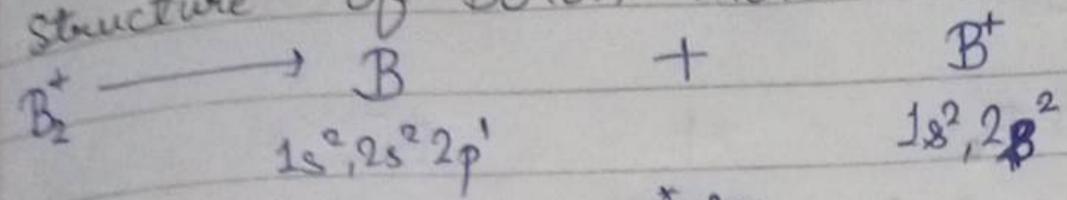
5) Structure of Boron molecule -



$$\text{Bond order} = \frac{N_b - N_a}{2} \rightarrow \frac{4 - 2}{2} \rightarrow 1 \quad [\text{B}-\text{B}]$$

Magnetic property \Rightarrow Due to presence of unpaired e^- in M.O. of B_2 . So it is a paramagnetic in nature.

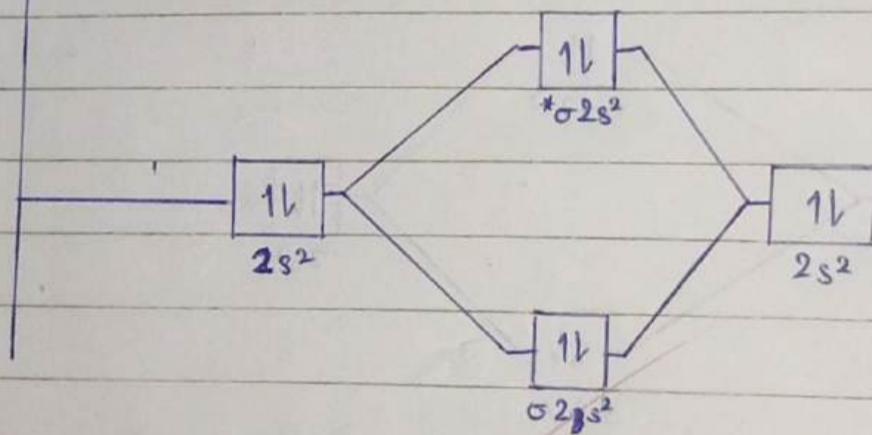
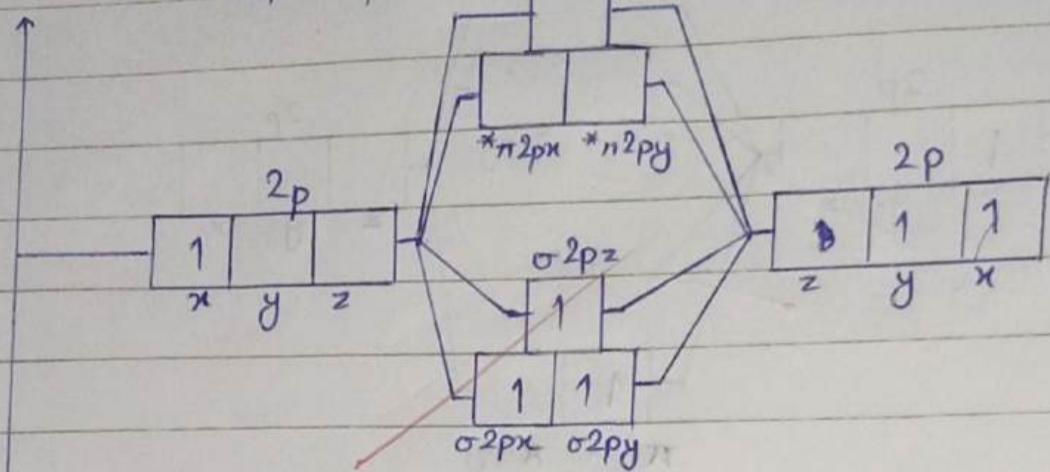
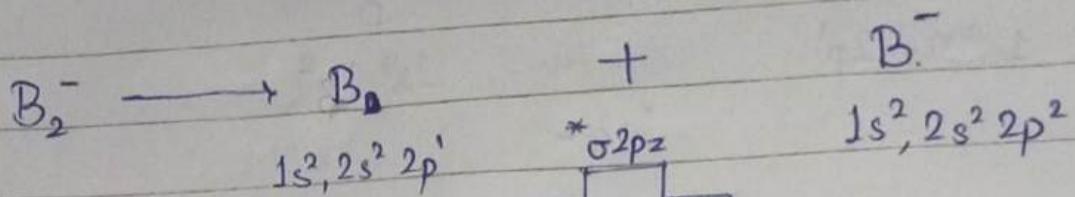
Structure of Boron molecule cation (B_2^+) -



$$\text{Bond order} = \frac{N_b - N_a}{2} \Rightarrow \frac{3-2}{2} \Rightarrow 0.5$$

Magnetic property \Rightarrow Due to presence of unpaired e^- in M.O. of B_2^+ . So it is a paramagnetic in nature.

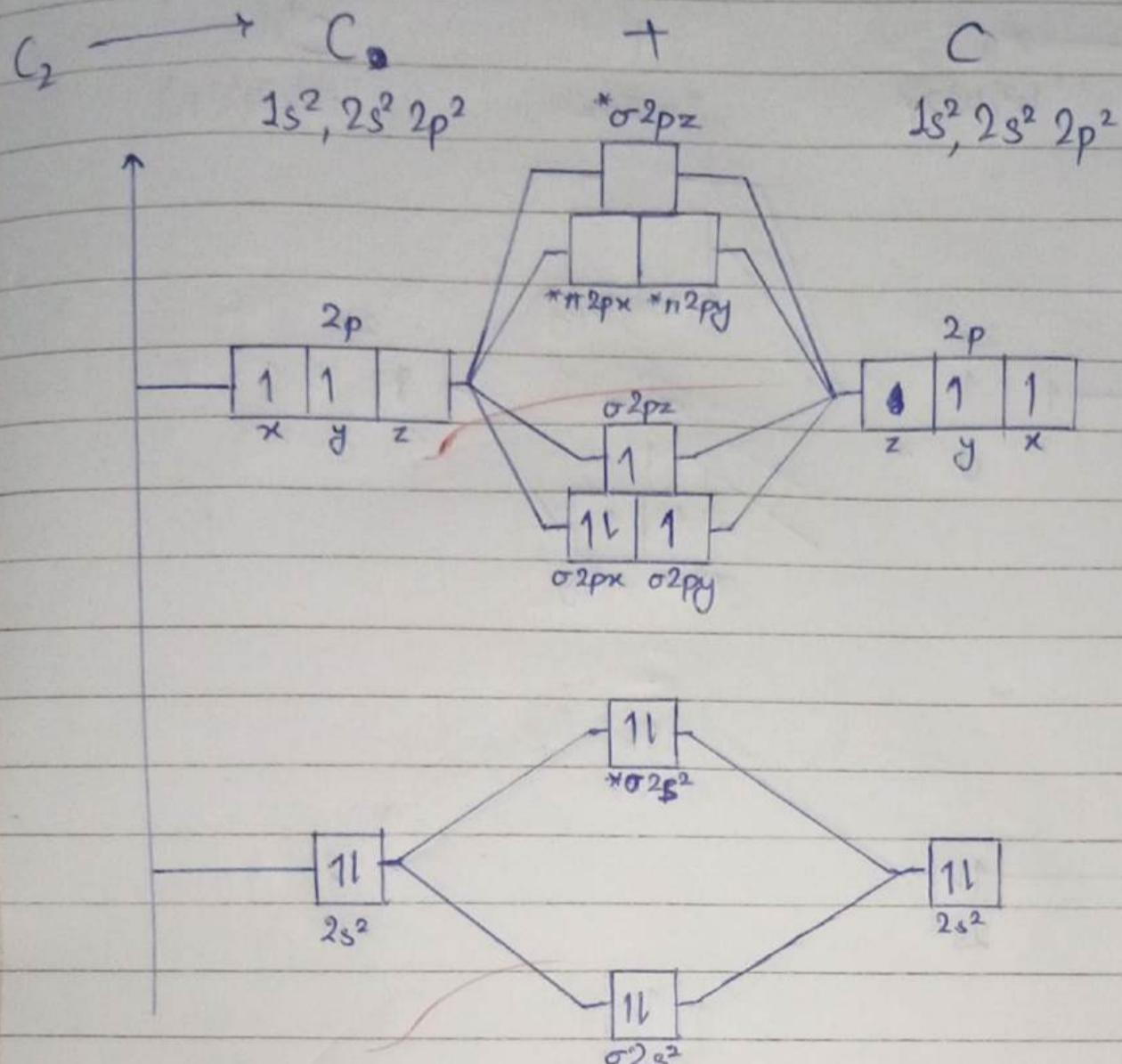
* Structure of Boron molecule anion (B_2^-) -



$$\text{Bond order} = \frac{N_b - N_a}{2} \Rightarrow \frac{5 - 2}{2} \Rightarrow 1.5$$

Magnetic property \Rightarrow Due to presence of unpaired e^- in M.O. of B_2^- . So it is para magnetic in nature.

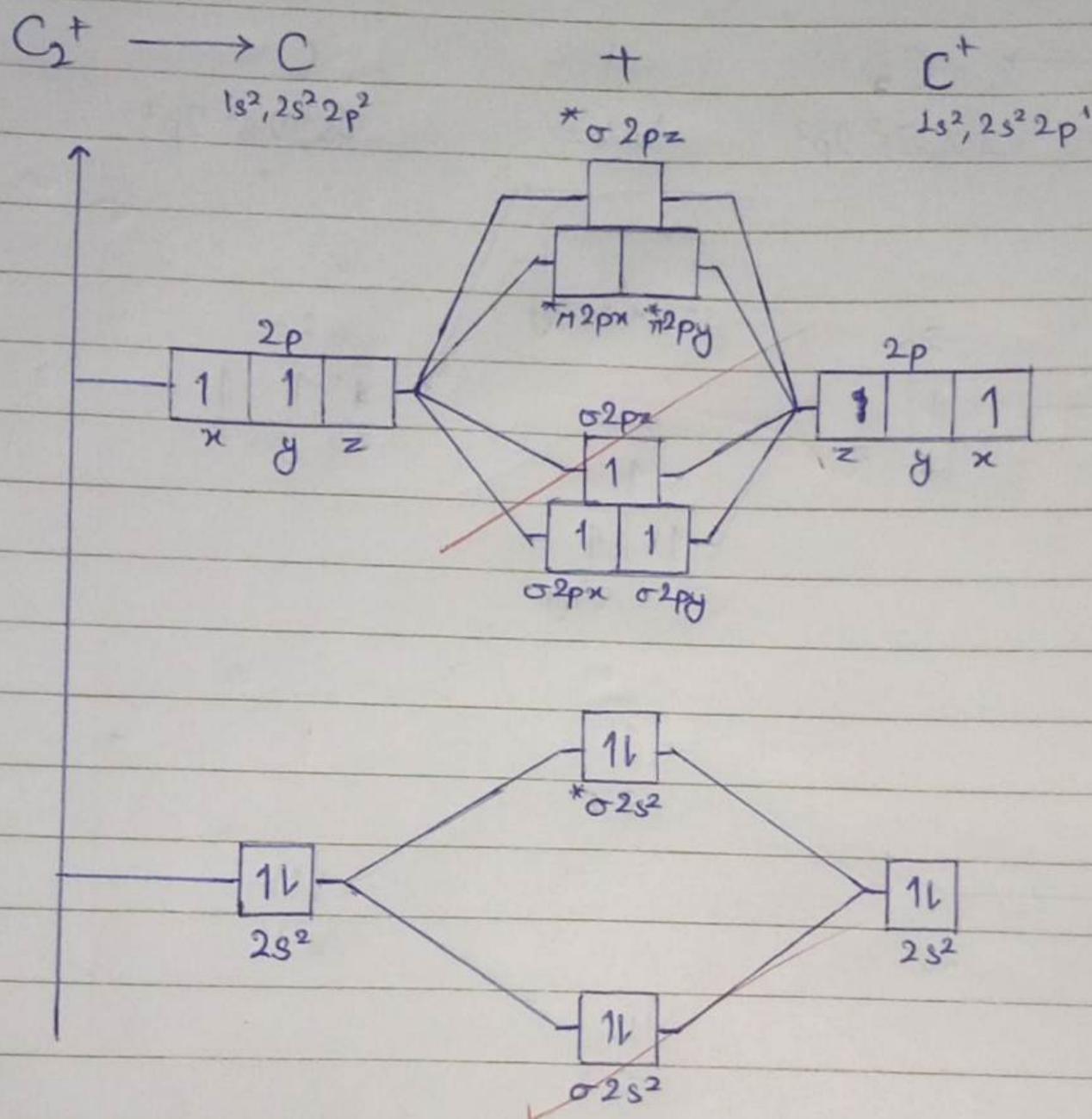
6) Structure of Carbon molecule -



$$\text{Bond order} = \frac{N_b - N_a}{2} \Rightarrow \frac{6 - 2}{2} \Rightarrow 2 [C=C]$$

Magnetic property \Rightarrow Due to presence of unpaired e^- in M.O. of C_2 . So it is para magnetic in nature.

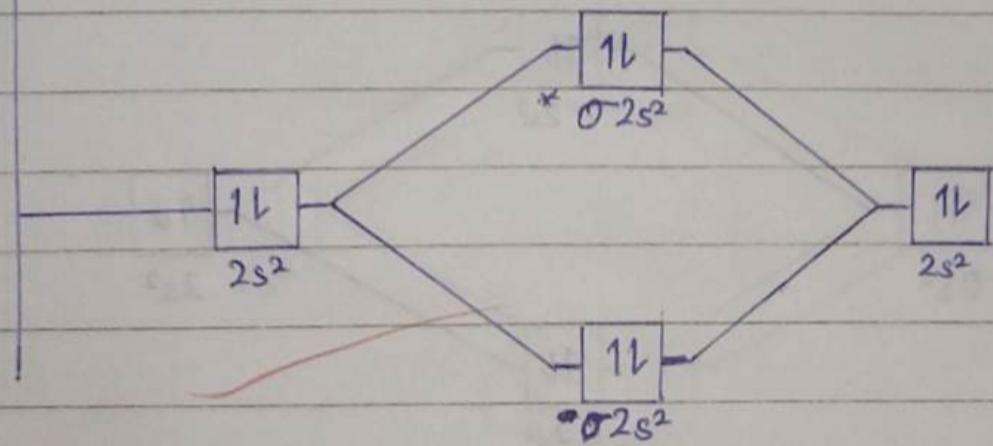
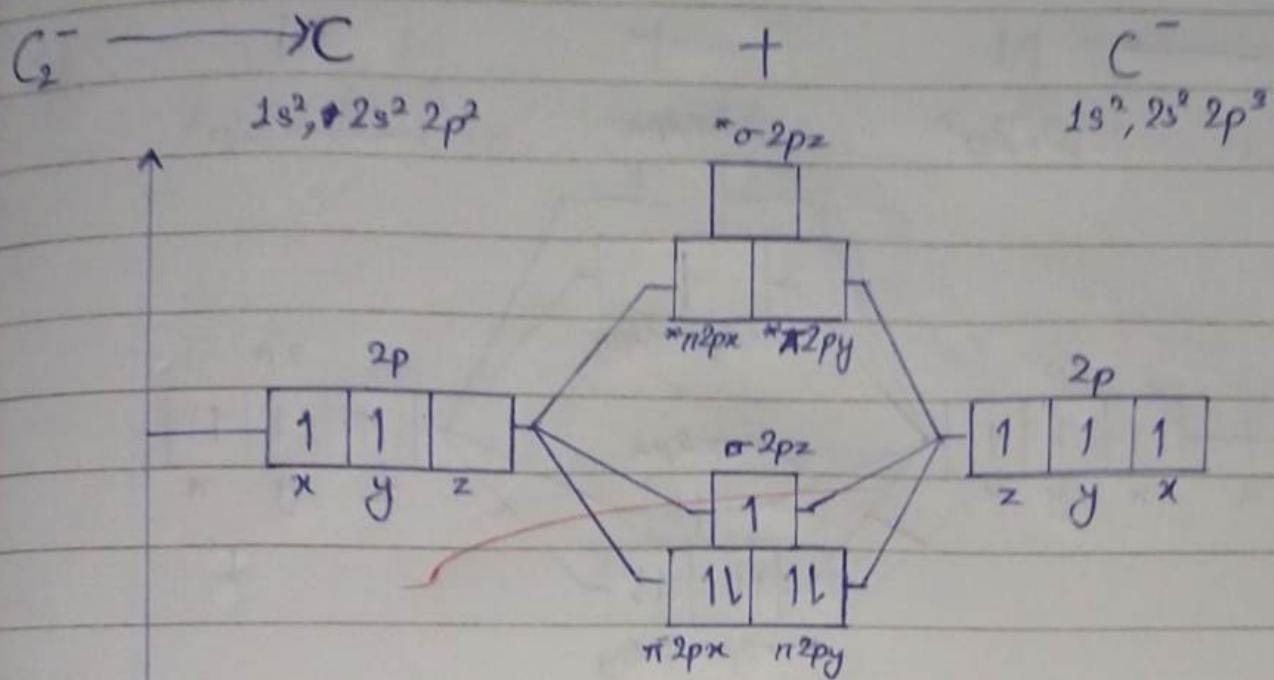
* Structure of carbon molecule cation (C_2^+) -



$$\text{Bond order} = \frac{N_b - N_a}{2} \Rightarrow \frac{5-2}{2} \Rightarrow 1.5$$

Magnetic property \Rightarrow Due to presence of unpaired e^- in M.O. of C_2^+ . So it is para magnetic in nature.

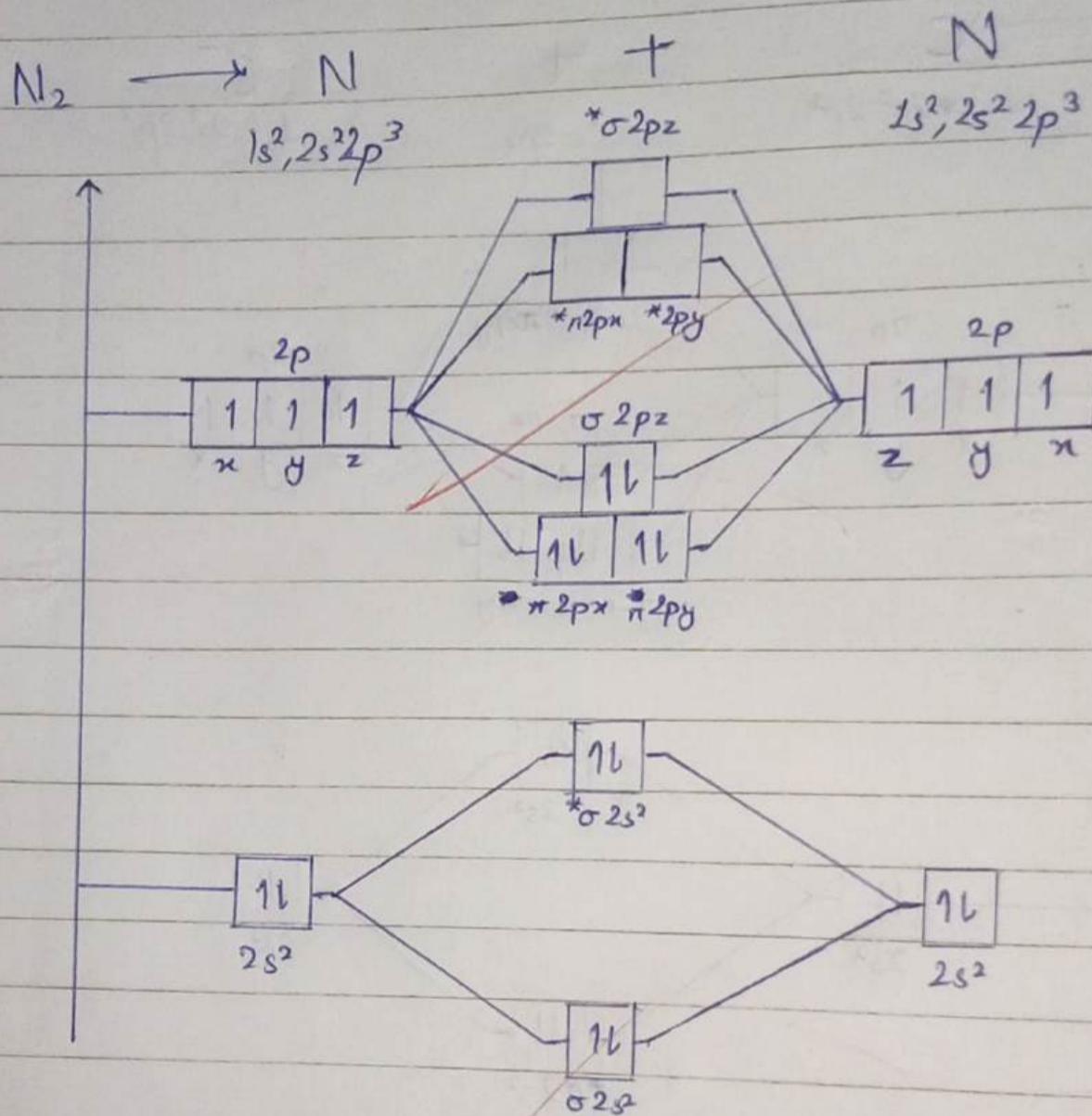
* Structure of Carbon molecule anion (C_2^-) -



$$\text{Bond order} = \frac{N_b - N_a}{2} \Rightarrow \frac{7 - 2}{2} \Rightarrow 2.5$$

Magnetic property \Rightarrow Due to presence of unpaired e^\ominus in M.O. of C_2^- . So it is paramagnetic in nature.

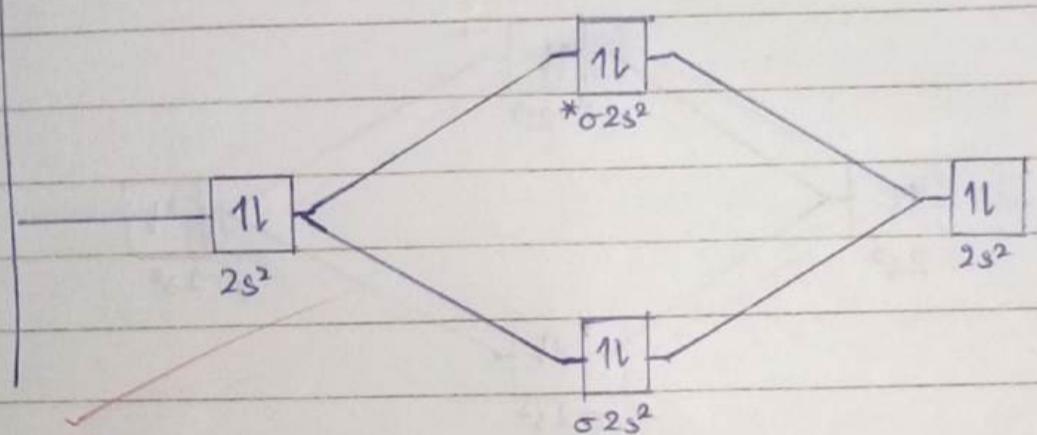
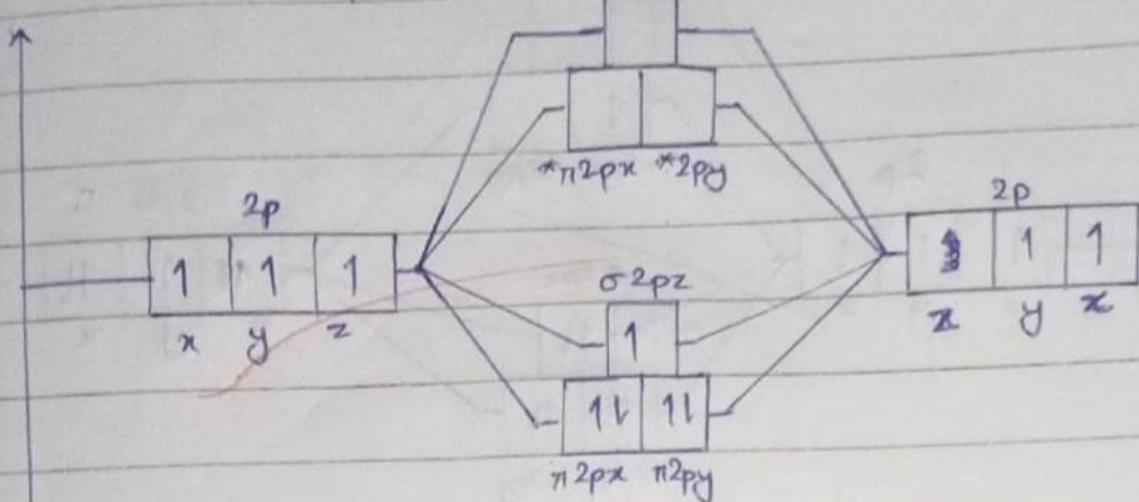
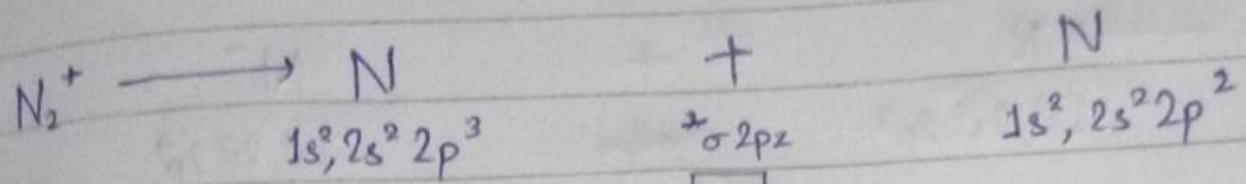
⇒ Structure of Nitrogen molecule -



$$\text{Bond order} = \frac{N_b - N_a}{2} \Rightarrow \frac{8 - 2}{2} \Rightarrow 3 \quad [N \equiv N]$$

Magnetic property \Rightarrow Due to presence of paired e^- in M.O. of N_2 . So it is diamagnetic in nature.

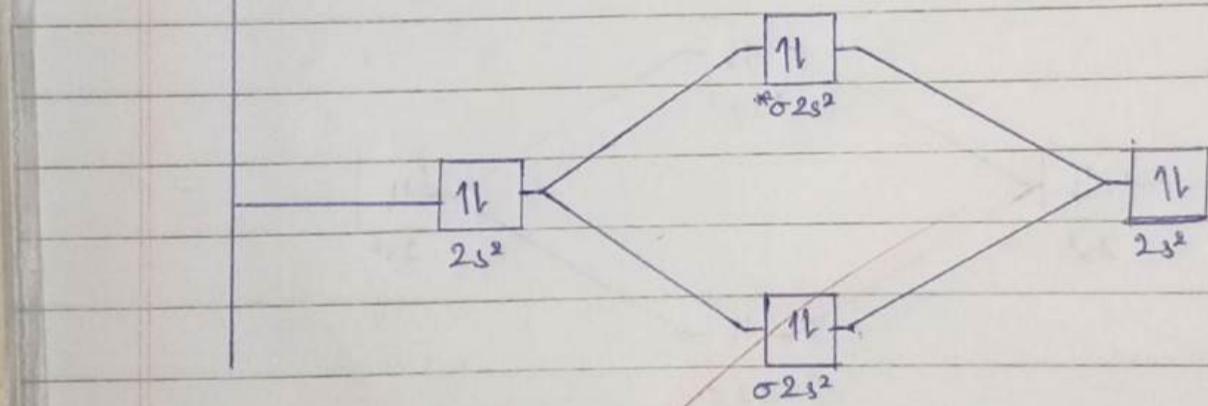
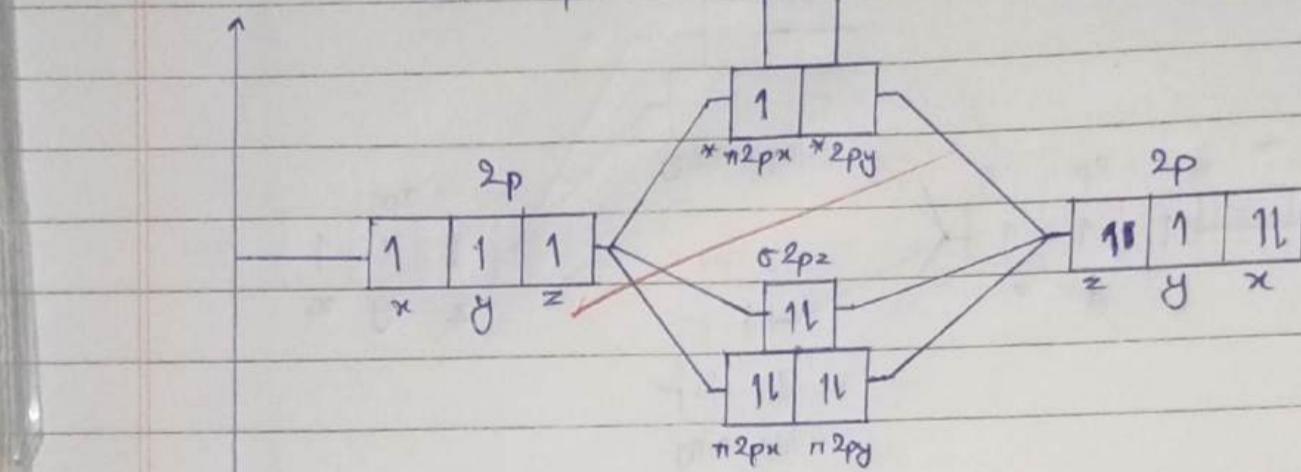
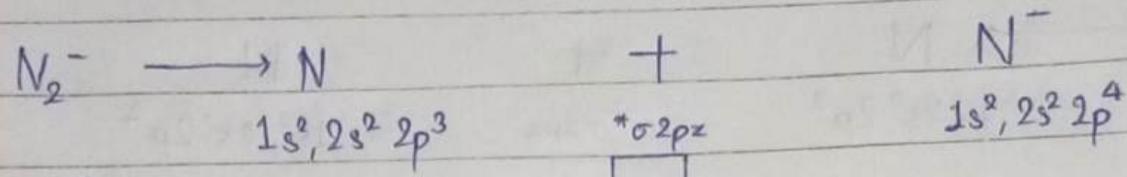
* Structure of Nitrogen molecule cation (N_2^+) -



$$\text{Bond order} = \frac{N_b - N_a}{2} \rightarrow \frac{7 - 2}{2} \Rightarrow 2.5$$

Magnetic property \Rightarrow Due to presence of unpaired e^- in M.O. of N_2^+ . So it is para magnetic in nature.

* Structure of Nitrogen molecule anion (N_2^-) -

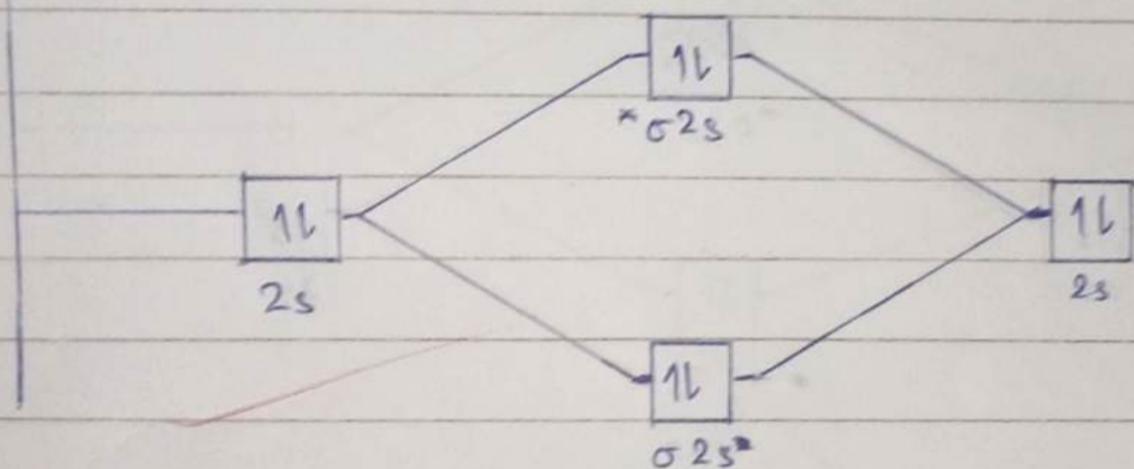
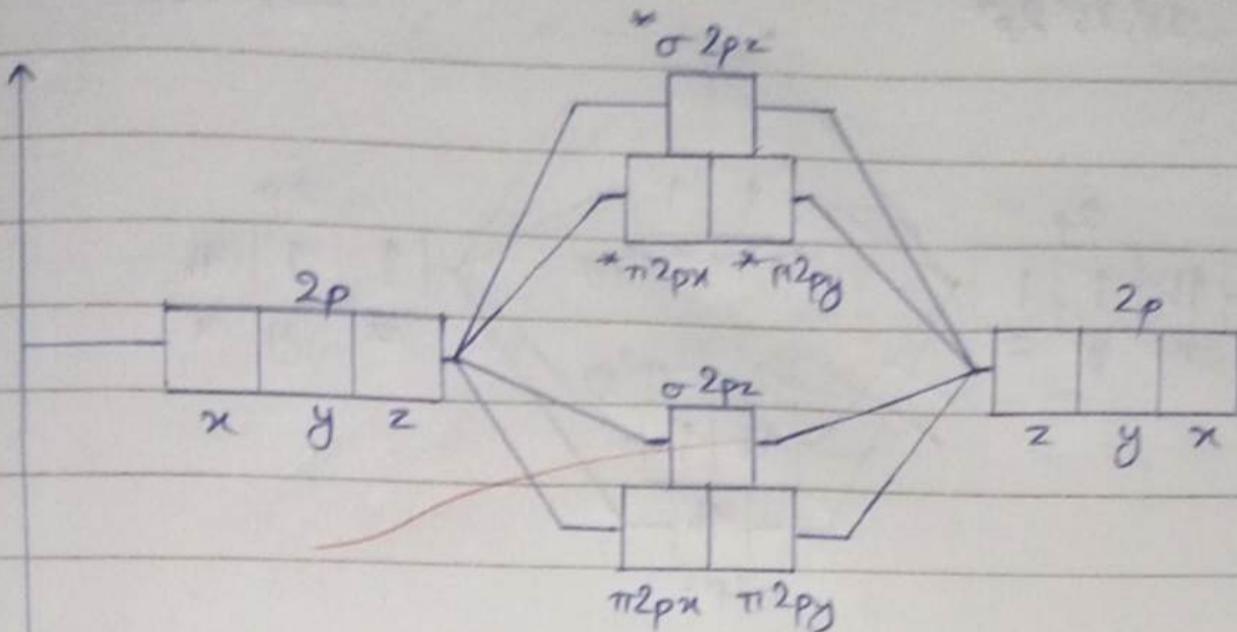


$$\text{Bond order} = \frac{N_b - N_a}{2} \Rightarrow \frac{8 - 3}{2} \Rightarrow 2.5$$

Magnetic property \Rightarrow Due to presence of unpaired of e^- in M.O. of N_2^- . So it is para magnetic in nature.

Bond
Mag.
 e^-
nat

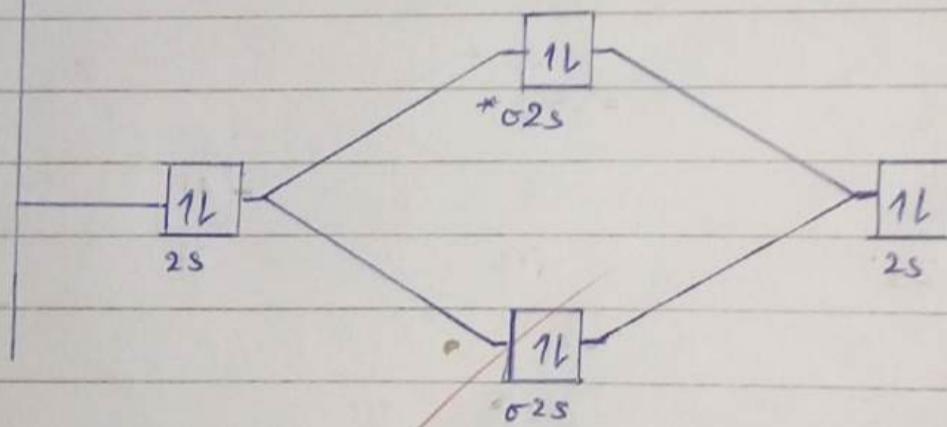
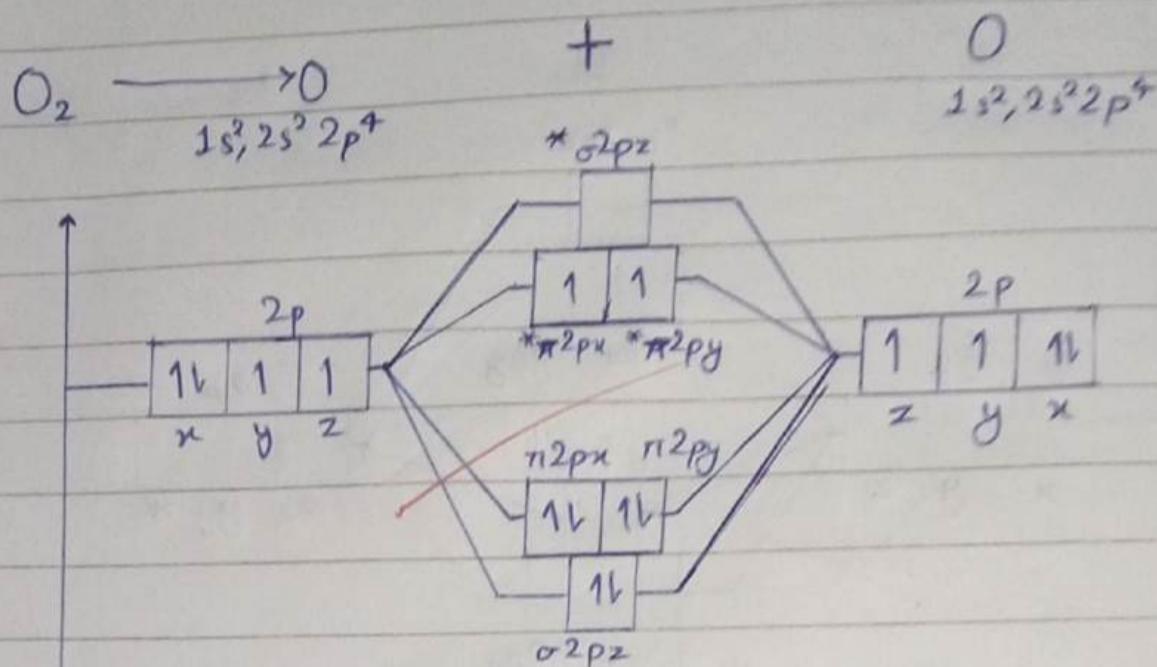
* Structure of



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

Magnetic property \Rightarrow Due to presence of unpaired e^\ominus in M.O. of N_2 . So, it is para magnetic in nature.

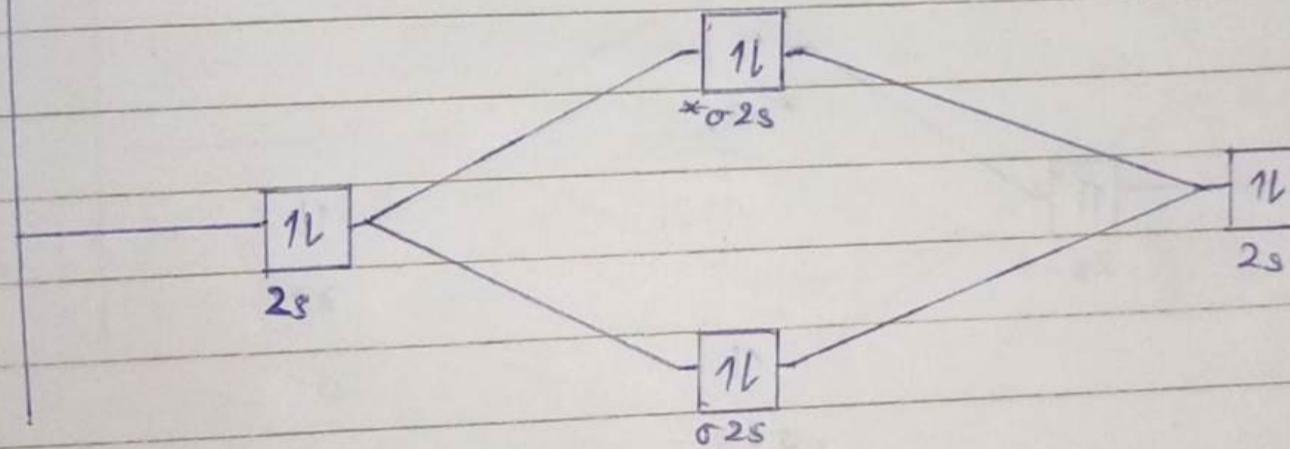
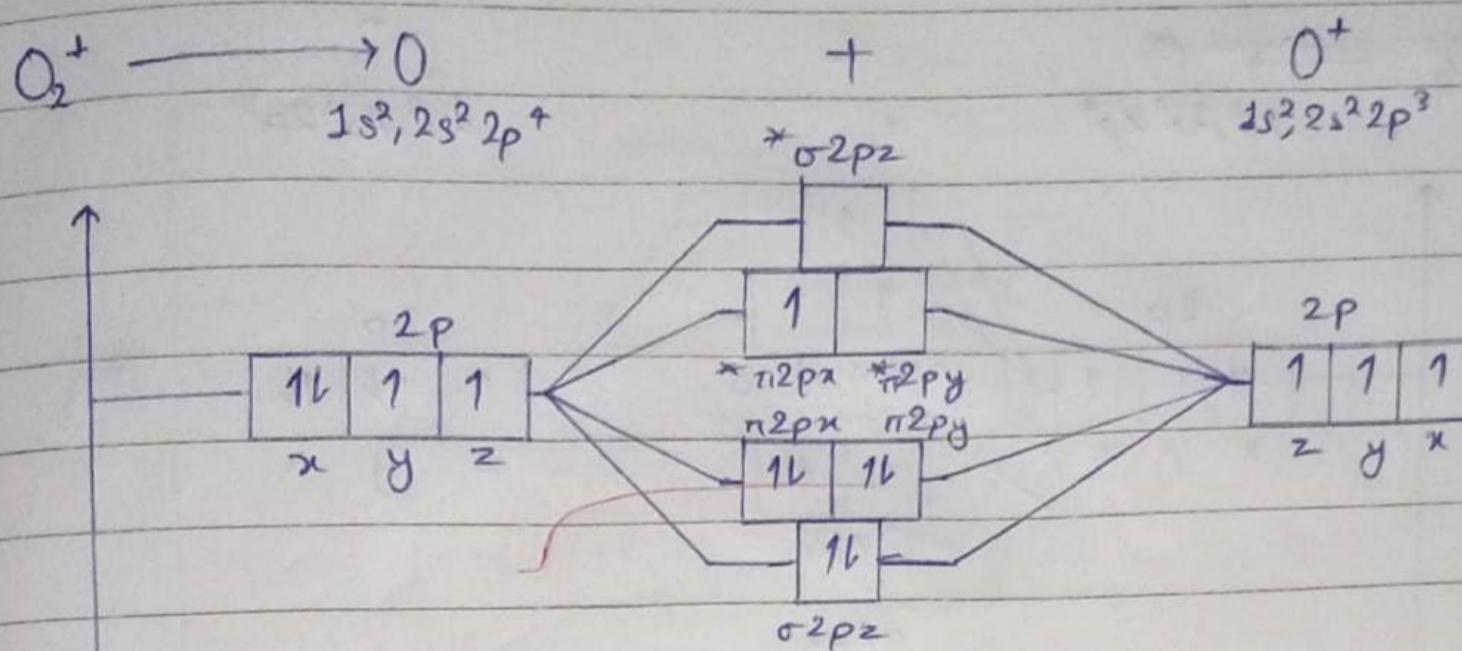
8) Structure of Oxygen molecule -



$$\text{Bond order} \Rightarrow \frac{N_b - N_a}{2} \Rightarrow \frac{8 - 4}{2} \Rightarrow 2 \quad [O=O]$$

Magnetic property \Rightarrow Due to presence of unpaired σ in M.O. of O_2 . So it is para magnetic in nature

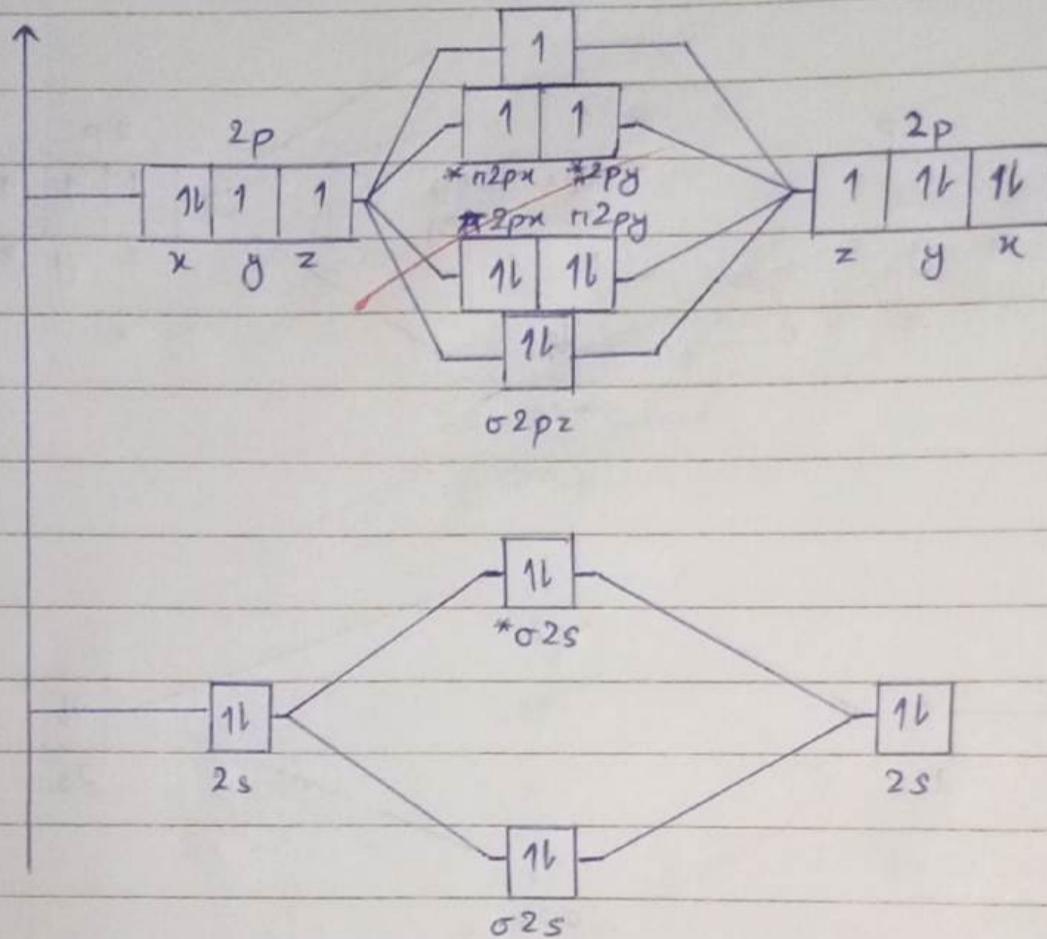
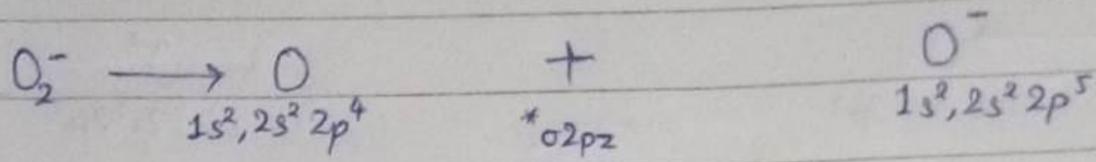
* Structure of Oxygen molecule cation (O_2^+) -



$$\text{Bond order} = \frac{N_b - N_a}{2} \Rightarrow \frac{8 - 3}{2} \Rightarrow 2.5$$

Magnetic property \Rightarrow Due to presence of unpaired e^- in M.O. of O_2^+ . So it is para magnetic in nature.

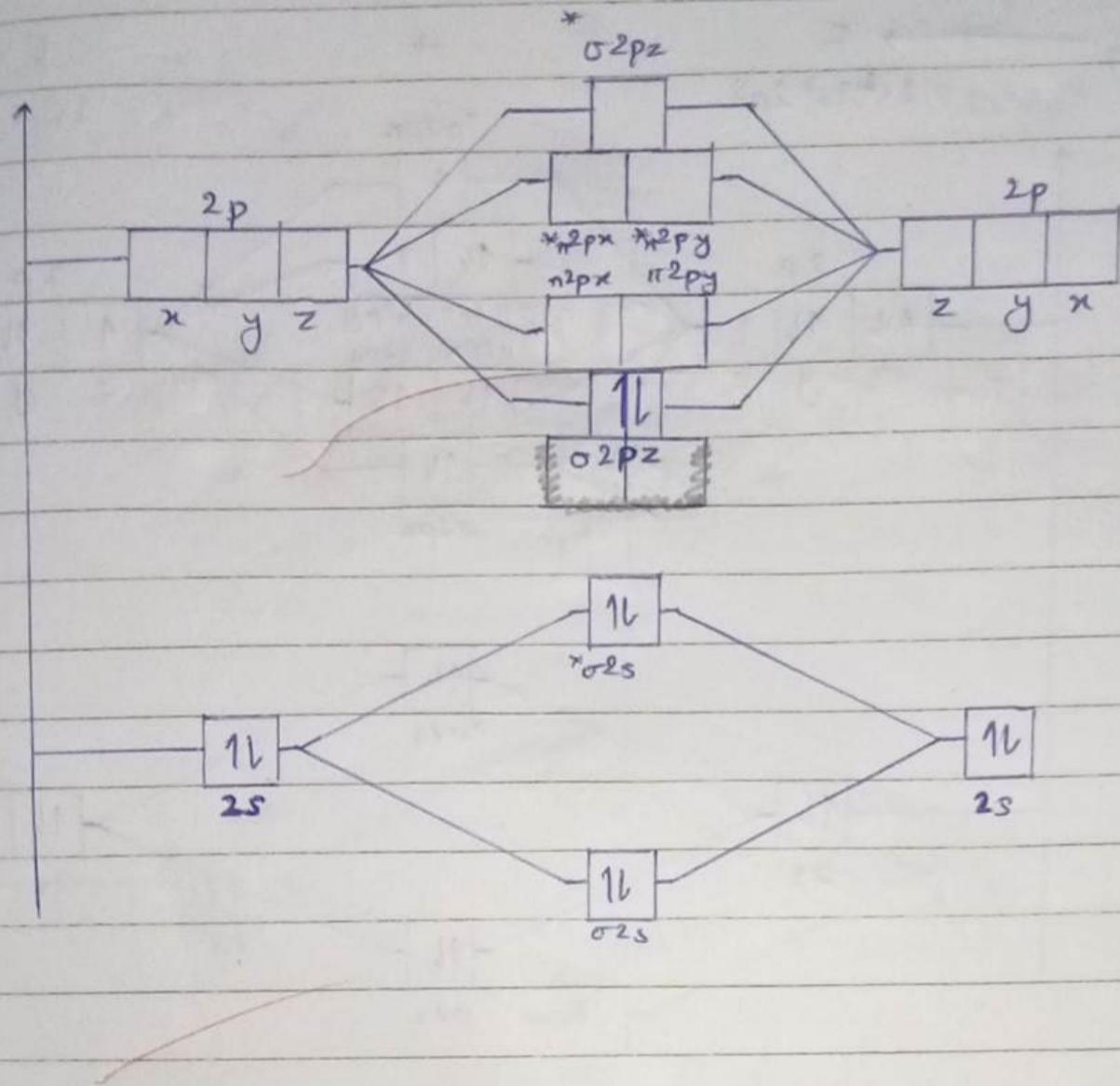
* Structure of Oxygen molecule anion (O_2^-) -



$$\text{Bond order} \rightarrow \frac{N_b - N_a}{2} \rightarrow \frac{8 - 5}{2} \rightarrow 1.5$$

Magnetic property \rightarrow Due to presence of unpaired e^- in M.O. of O_2^- . So it is paramagnetic in nature.

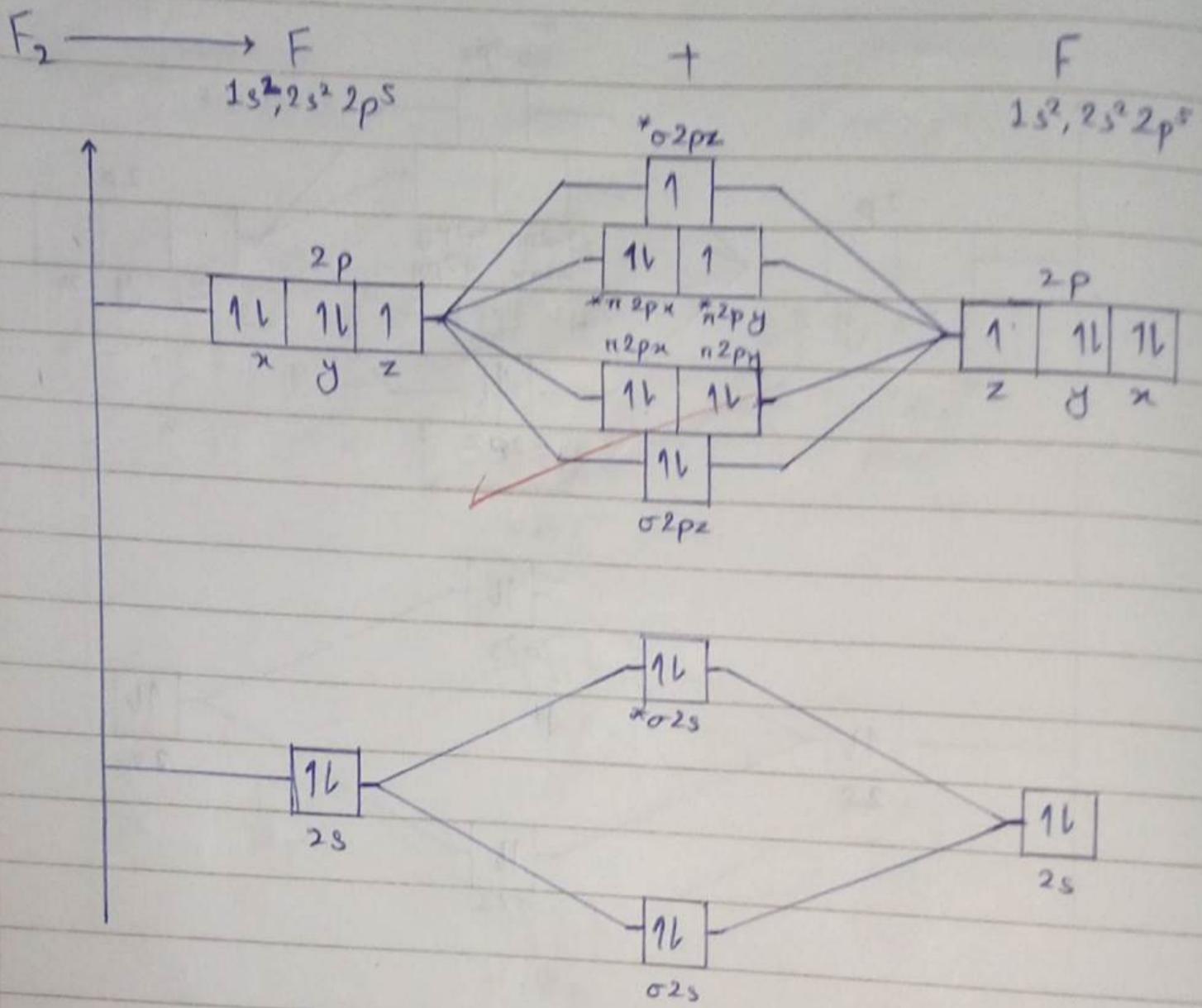
* Structure of



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

Magnetic property \Rightarrow Due to presence of unpaired e^- in M.O. of O_2 . So it is paramagnetic in nature.

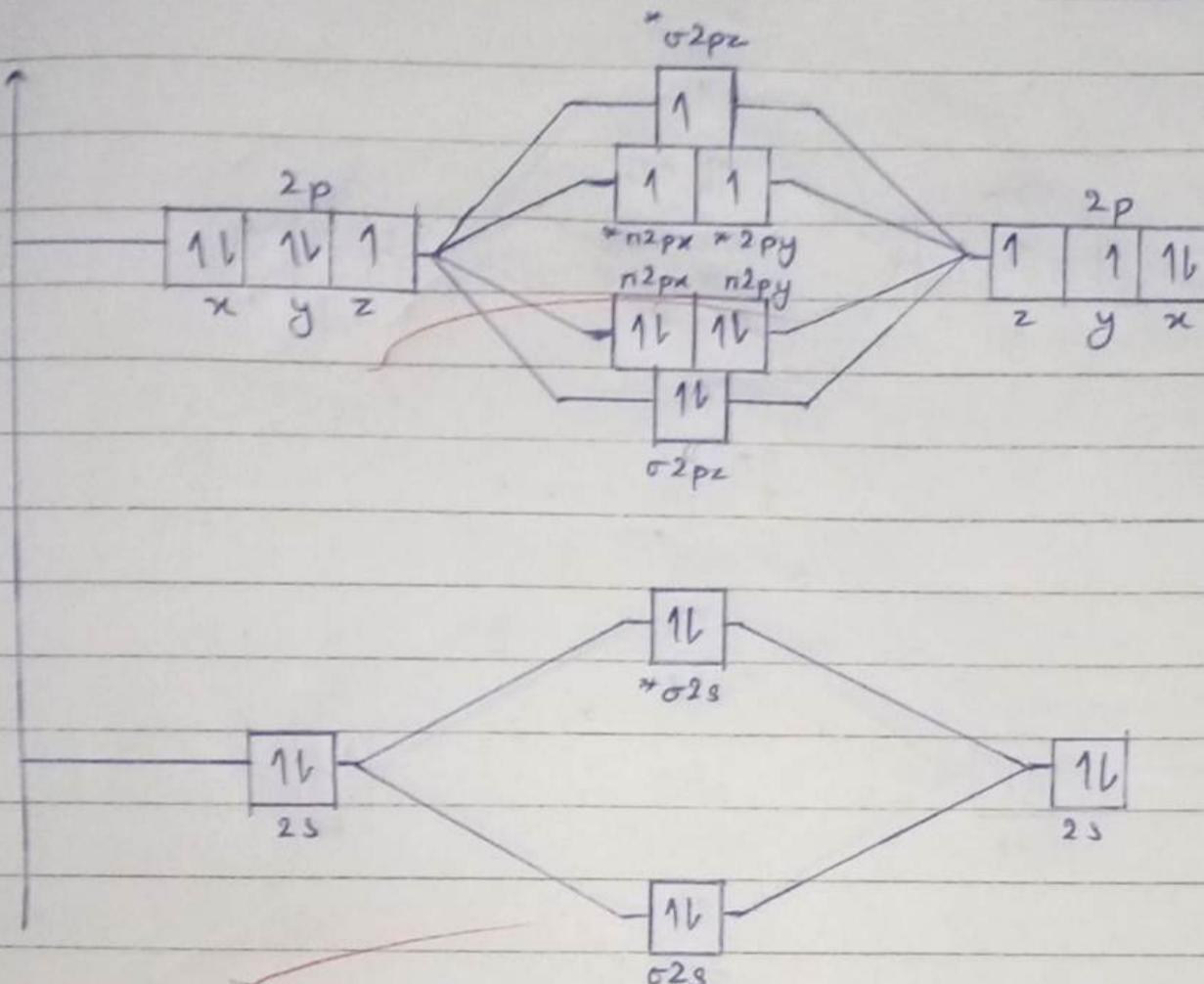
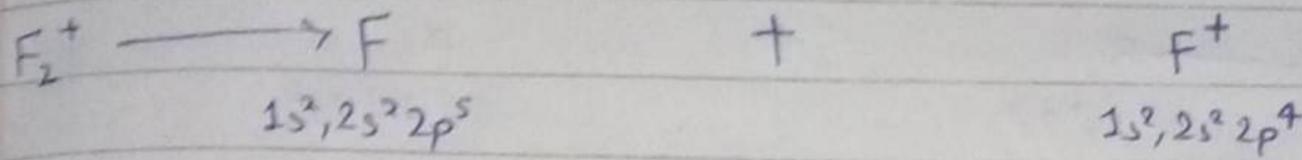
Q) Structure of Fluorine molecule



$$\text{Bond order} = \frac{N_b - N_a}{2} \Rightarrow \frac{8 - 6}{2} \Rightarrow 1 \quad [F - F]$$

Magnetic property \Rightarrow Due to presence of unpaired e^- in M.O. of F_2 . So it is paramagnetic in nature.

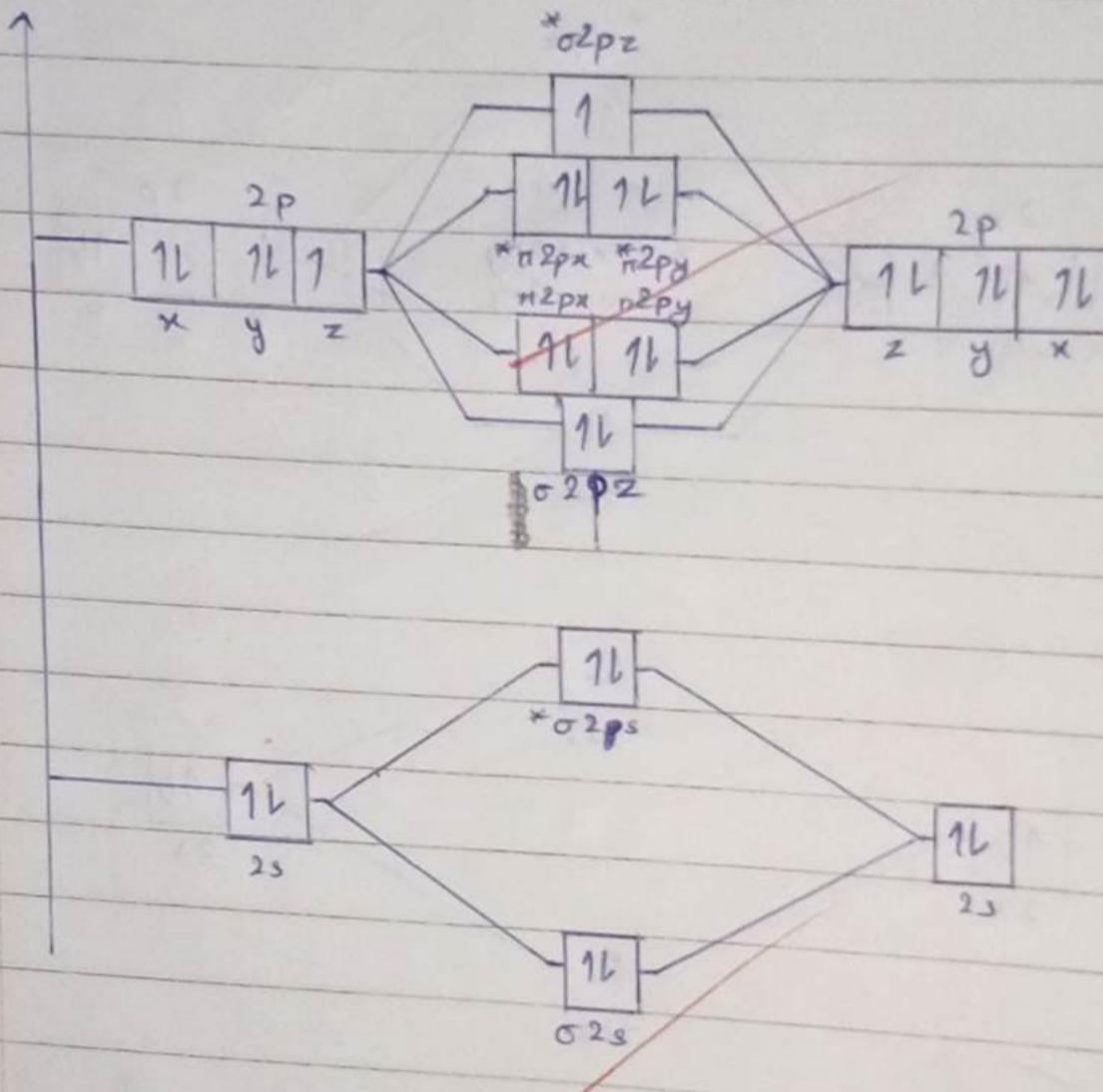
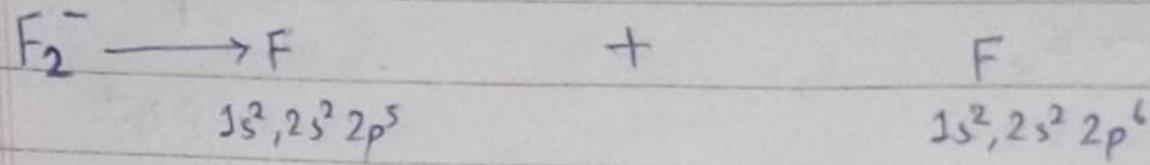
* Structure of Fluorine molecule cation (F_2^+)



$$\text{Bond order} = \frac{N_b - N_a}{2} \Rightarrow \frac{8 - 5}{2} \Rightarrow 1.5$$

Magnetic property \Rightarrow Due to presence of unpaired e^- in M.O. of F_2^+ . So it is para magnetic in nature.

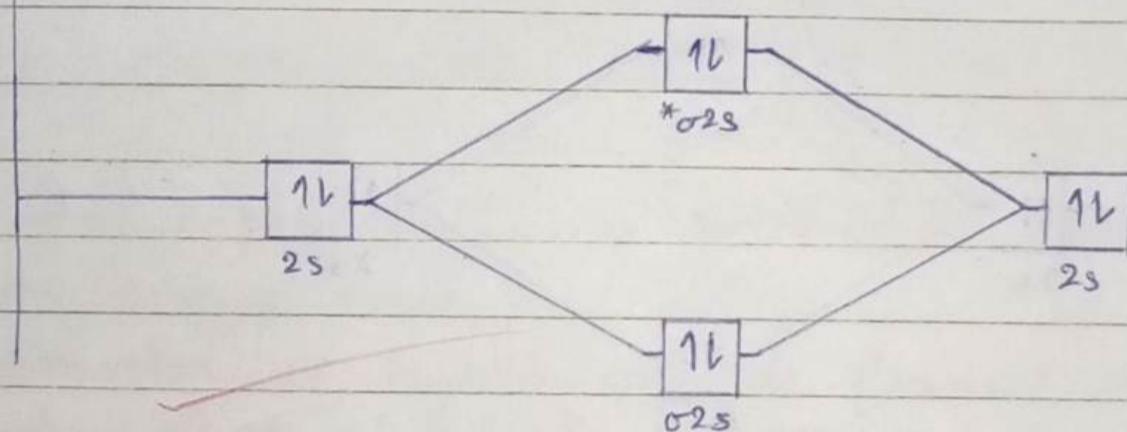
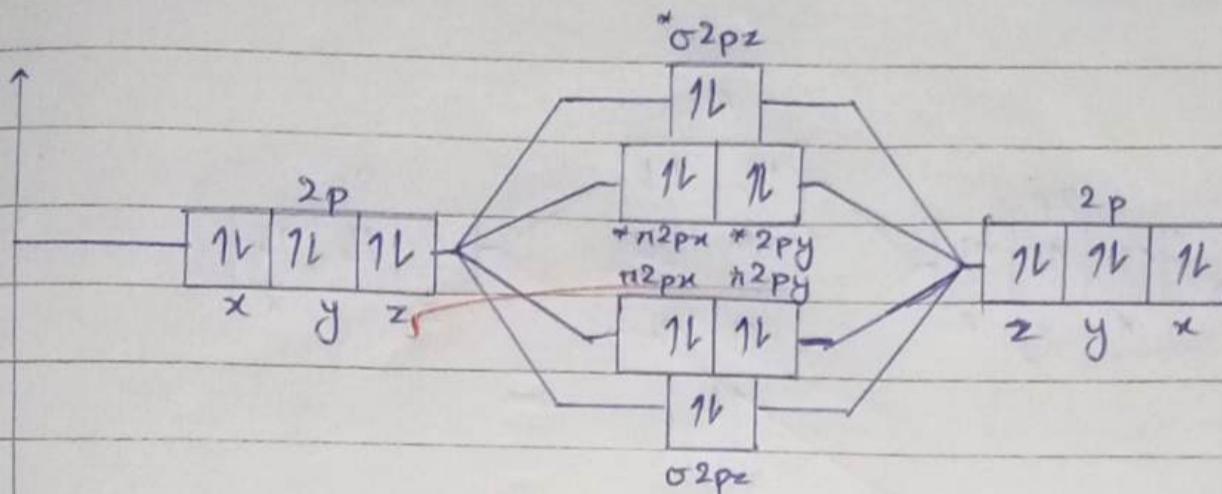
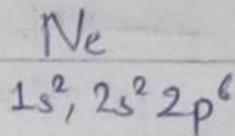
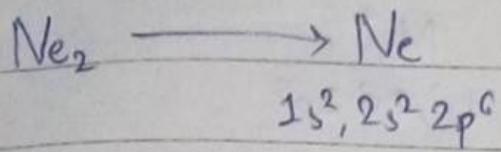
* Structure of Fluorine molecule anion (F_2^-) -



$$\text{Bond order} \Rightarrow \frac{N_b - N_a}{2} = \frac{8 - 7}{2} = 0.5$$

Magnetic property \Rightarrow Due to presence of unpaired e^- in M.O. of F_2^- . So it is paramagnetic in nature.

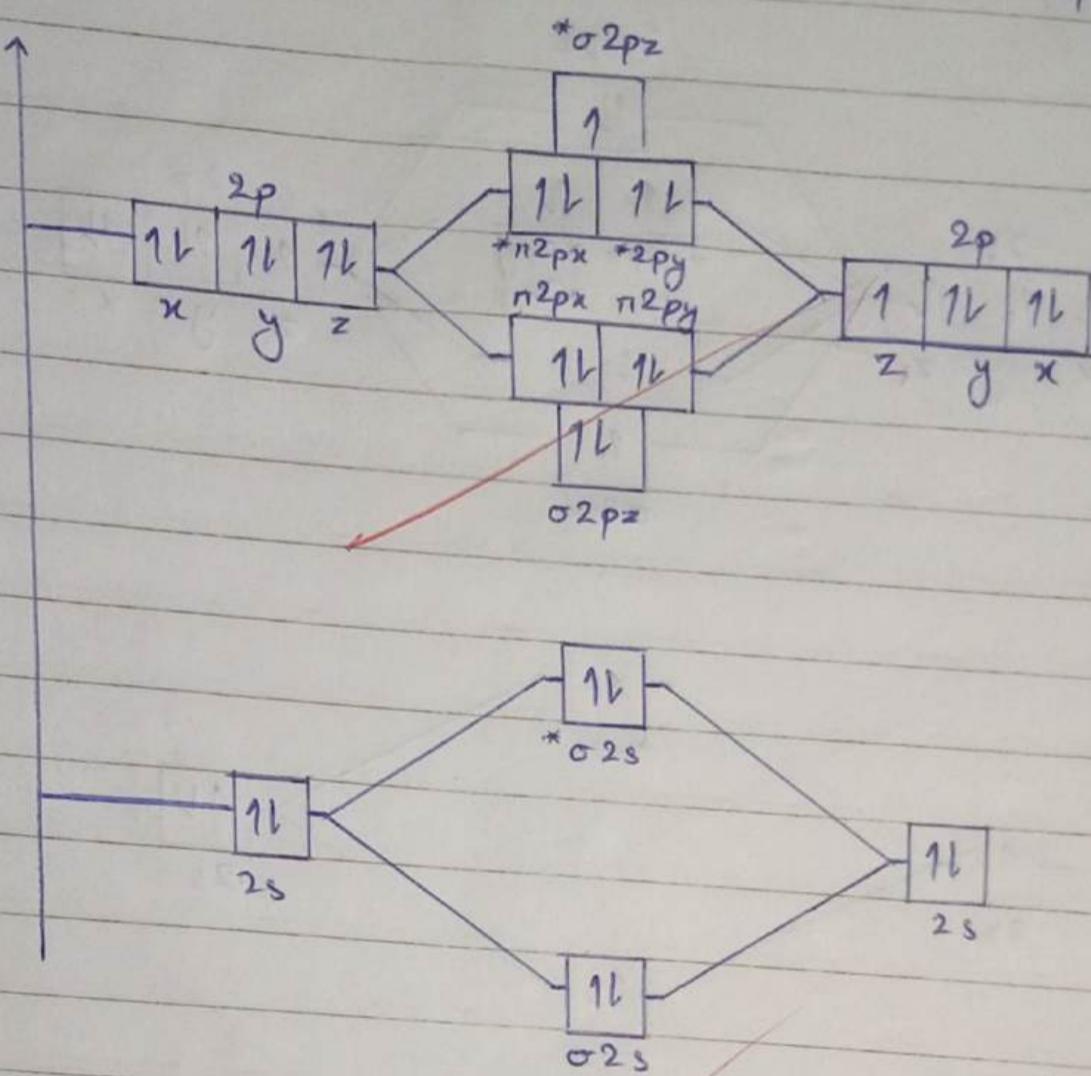
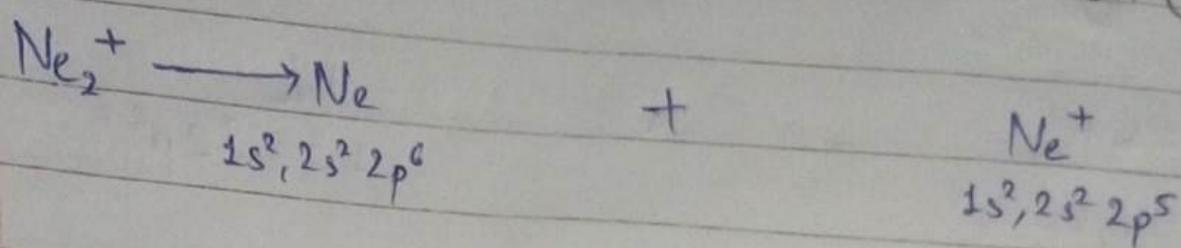
10) Structure of Neon molecule -



$$\text{Bond order} = \frac{N_b - N_a}{2} \Rightarrow \frac{8 - 8}{2} = 0$$

Magnetic property \Rightarrow Due to presence of paired e^\ominus in M.O of Ne_2 . So it is di magnetic in nature.

* Structure of Neon molecule anion (Ne_2^+) -



Bond order $\Rightarrow \frac{\text{No. of bonding MOs} - \text{No. of antibonding MOs}}{2} \Rightarrow \frac{8 - 7}{2} = 0.5$

Magnetic property \Rightarrow Due to presence of unpaired e^- in M.O. of Ne_2^+ . So it is para magnetic in nature.

Concept of Hybridisation

The process of mixing atomic orbitals of nearly the same energy and different shape to form equal number of new orbitals of same energy and shape is called hybridisation.

Valency of Be should be zero, 1 of B and 2 of C but in actual, valency of Be is 2, B is 3 and that of C is 4. The reason for this, that has been suggested is that some paired electrons get excited to the vacant orbitals by taking energy.

Rules of Hybridisation

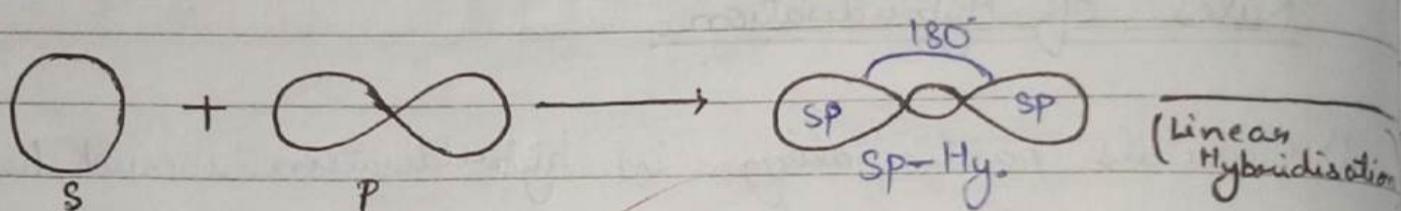
- 1) Orbitals participating in hybridisation should be of almost same energy levels.
- 2) The number of hybrid orbitals formed are equal to the number of p orbitals participating in it.
- 3) Orbitals (not electrons) participate in hybridisation. Therefore orbitals that participate in hybridisation can be half filled, completely filled or vacant.
- 4) Excitation of electron is not necessary for hybridisation.
- 5) Hybrid orbitals are similar in energy and shape but have different orientations in space. Orientation provides minimum repulsion between orbitals.
- 6) Hybridisation depends upon chemical atmosphere, e.g., in C_2H_6 , C_2H_4 , C_2H_2 etc. each carbon atom is related respectively with 3, 2, 1 hydrogen atoms therefore all the three have sp^3 , sp^2 , sp hybridisation respectively.

- 7) Redistribution of energy and charge takes place in hybridisation.
- 8) The bonds formed by hybrid orbitals are comparatively stronger.

Types of Hybridisation

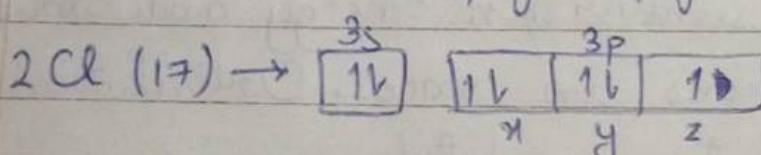
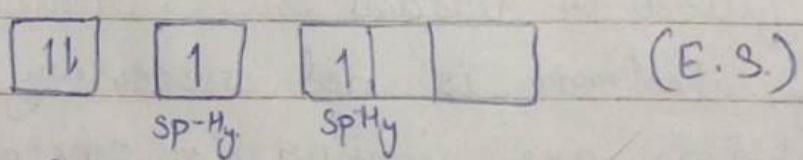
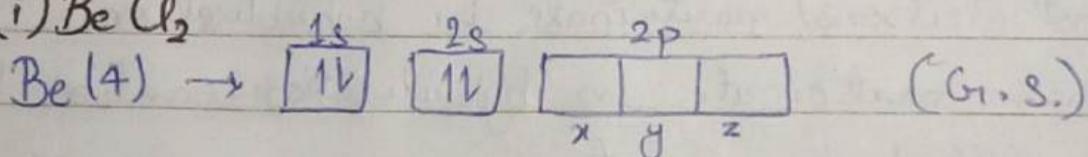
1) ~~sp-Hybridisation (Linear or Diagonal Hybridisation)~~

When one s- and one p-orbital combine to form two linear sp-hybrid orbitals of equal energies which are inclined to each other at an angle of 180° then it is called sp-hybridisation.

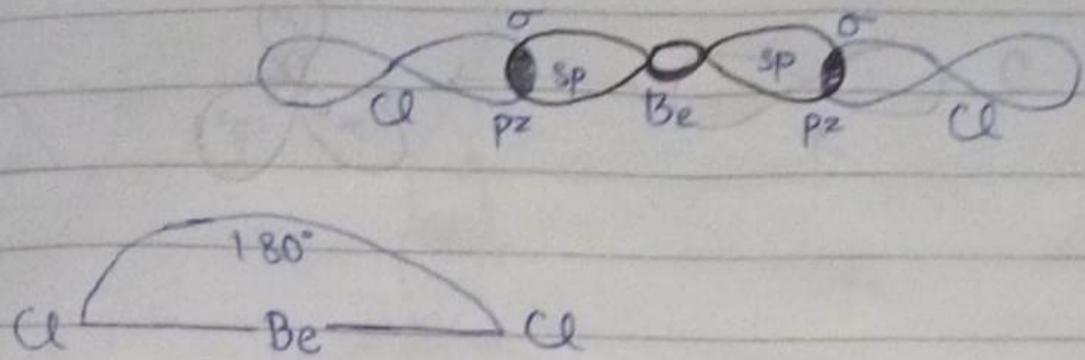
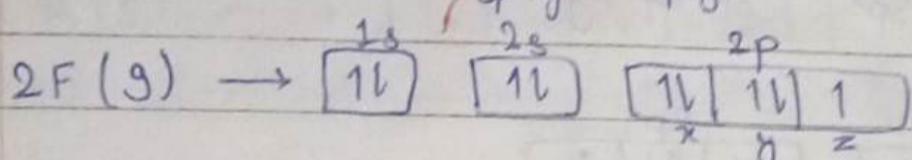
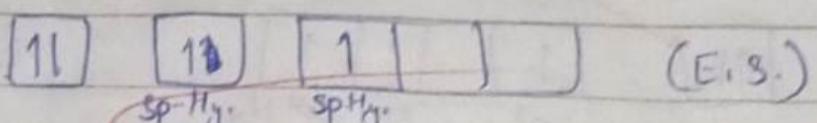
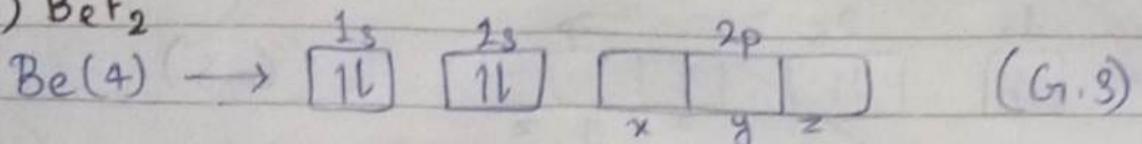


Example →

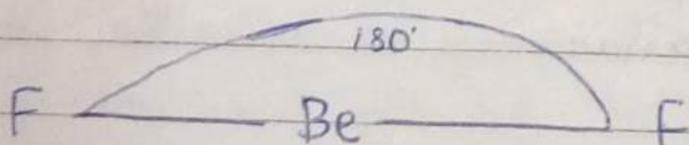
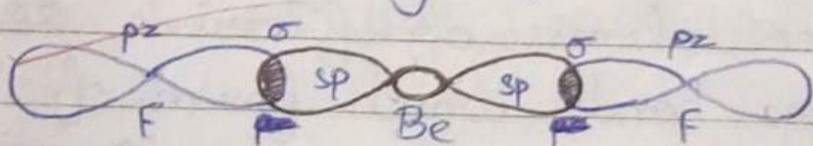
(i) BeCl_2



Two sp-hybrid orbitals are formed after hybridisation in $2s$ and $2p_x$ orbitals which contain single unpaired electron. These hybridised orbitals undergo co-axial overlapping with p-orbital of Chlorine to form sp-p sigma bond. sp-p hybrid orbitals are inclined at angle of 180° to each other and the geometry of BeCl_2 molecule is linear.

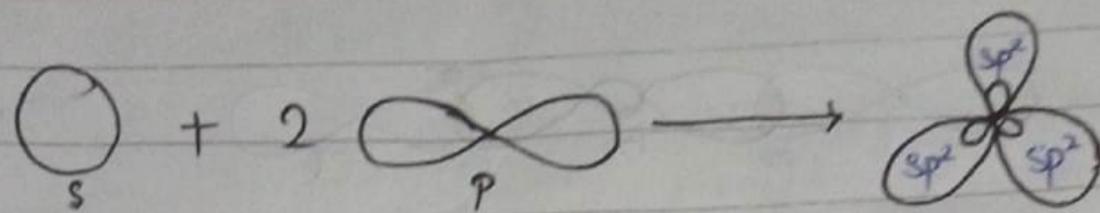
(ii) BeF_2 

Two sp-hybrid orbitals are formed after hybridisation in 2s and 2p_x orbitals which contain single unpaired electron. These hybridised orbitals undergo co-axial overlapping with p-orbital of Fluorine to form sp-p sigma bond. sp-p hybrid orbital are inclined at angle of 180° to each other and the geometry of BeF_2 molecule is linear.



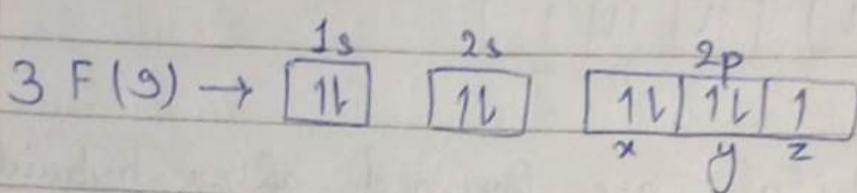
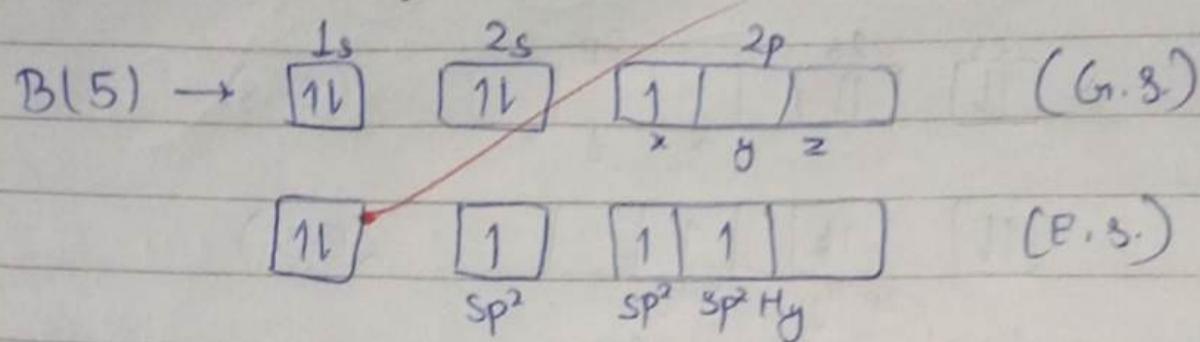
2) sp^2 - Hybridisation (Trigonal Hybridisation)

In this one s- and two p-orbitals combine to form three sp^2 -hybrid orbitals which are coplanar and form 120° angle with each other. This type of hybridisation is called Trigonal hybridisation. As a result, central atom of the molecules is in sp^2 -hybridised state and they are trigonally coplanar.



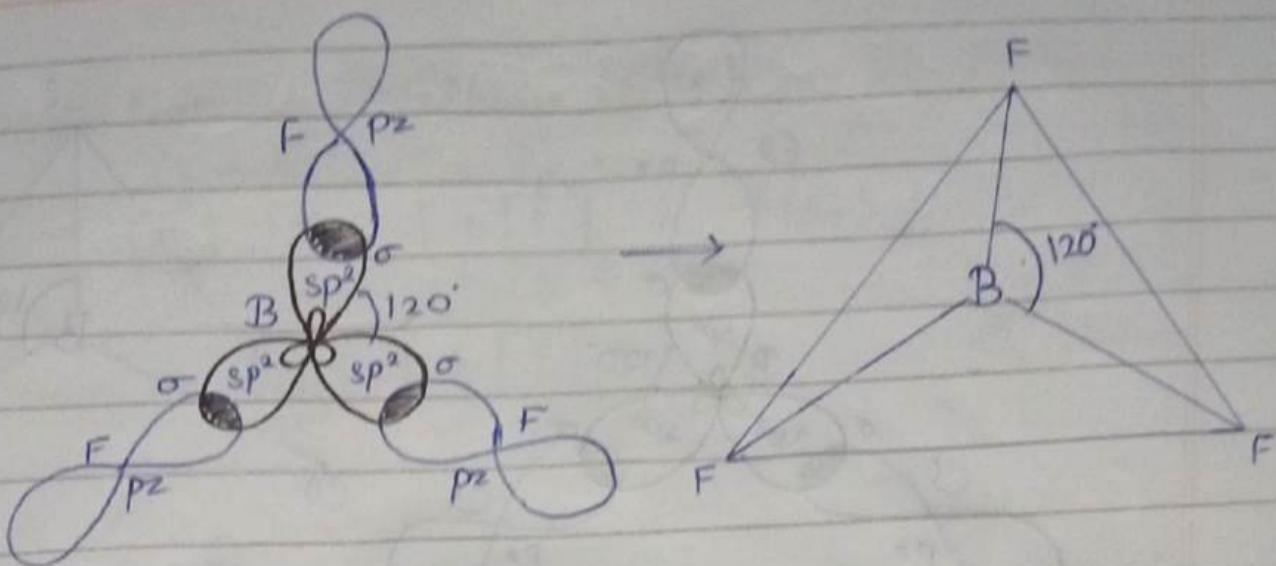
Example →

(i) Formation of BF_3 →

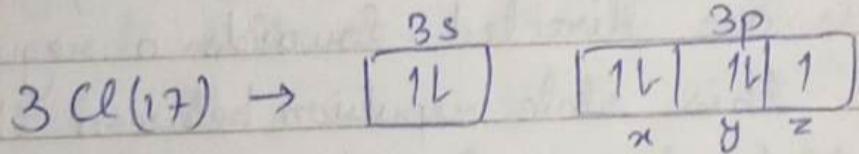
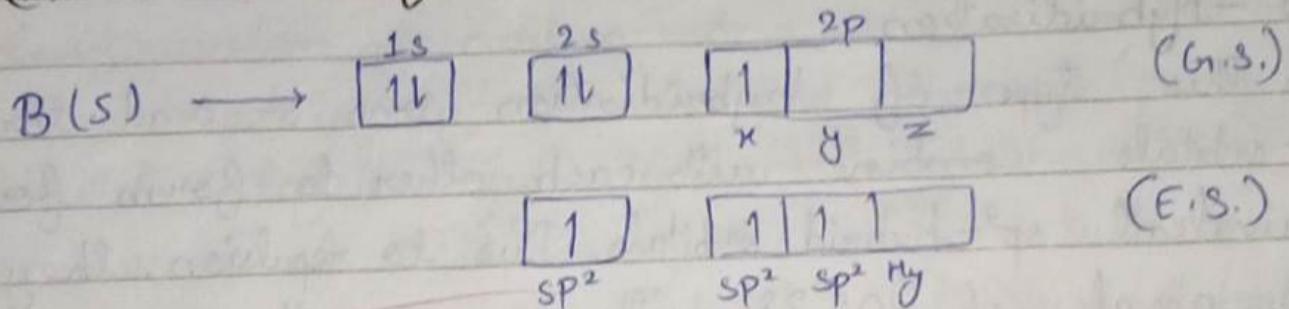


Central atom of BF_3 is boron. In excited state its configuration is $1s^2, 2s^1, 2p_x^1, 2p_y^1$. Its one s- and two p ($2p_x$ and $2p_y$)-orbitals hybridise to form three sp^2 -hybrid orbitals.

This boron atom undergoes sp^2 -p overlapping with three atoms of fluorine to form three sp^2 -p sigma bonds which form of 120° with each other in one plane. As a result, BF_3 molecule is Trigonal planar.

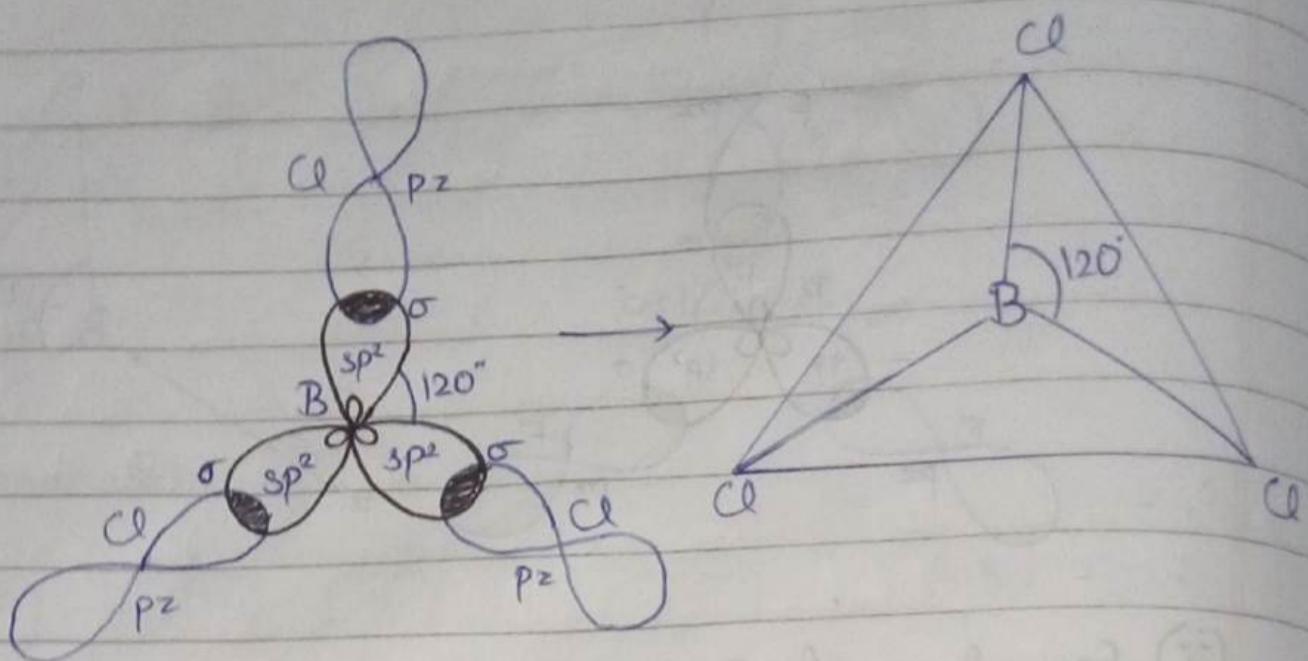


(ii) Formation of $\text{BCl}_3 \rightarrow$



Central atom of BCl_3 is boron. In excited state its configuration is $1\text{s}^2, 2\text{s}^1, 2\text{p}_x^1, 2\text{p}_y^1$. Its one s- and two p (2p_x and 2p_y) - orbitals hybridise to form three sp^2 - hybrid orbitals.

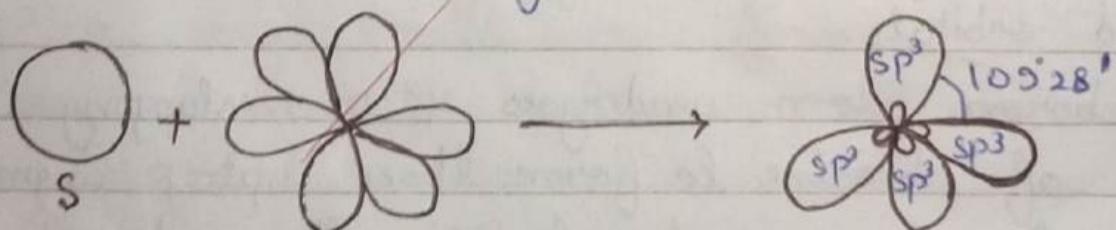
This boron atom undergoes sp^2-p overlapping with three atoms of chlorine to form three sp^2-p sigma bonds which form an angle of 120° with each other in one plane. As a result, BCl_3 molecule is Trigonal planar.



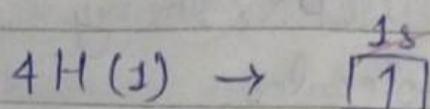
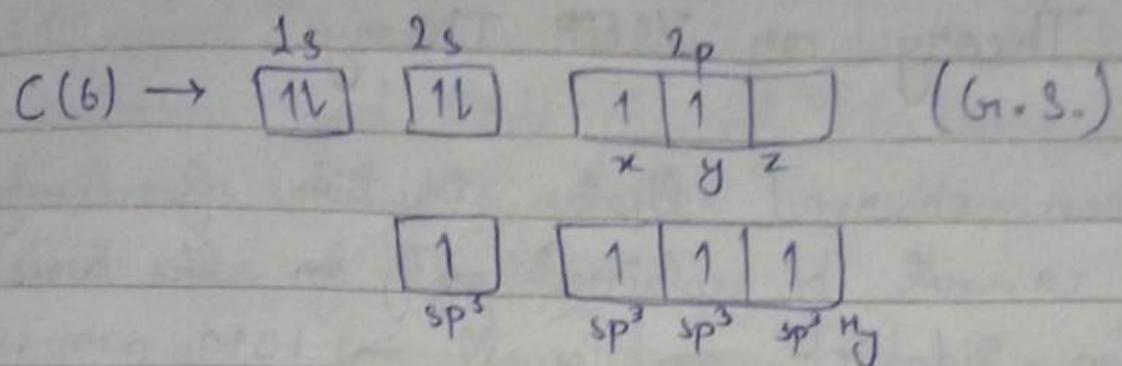
3) sp^3 -Hybridisation

In this type of hybridisation one s- and three p-orbitals combine with each other to form four equivalent sp^3 -hybrid orbitals. Due to repulsion, they form an angle of $109^{\circ}28'$ with one another in space.

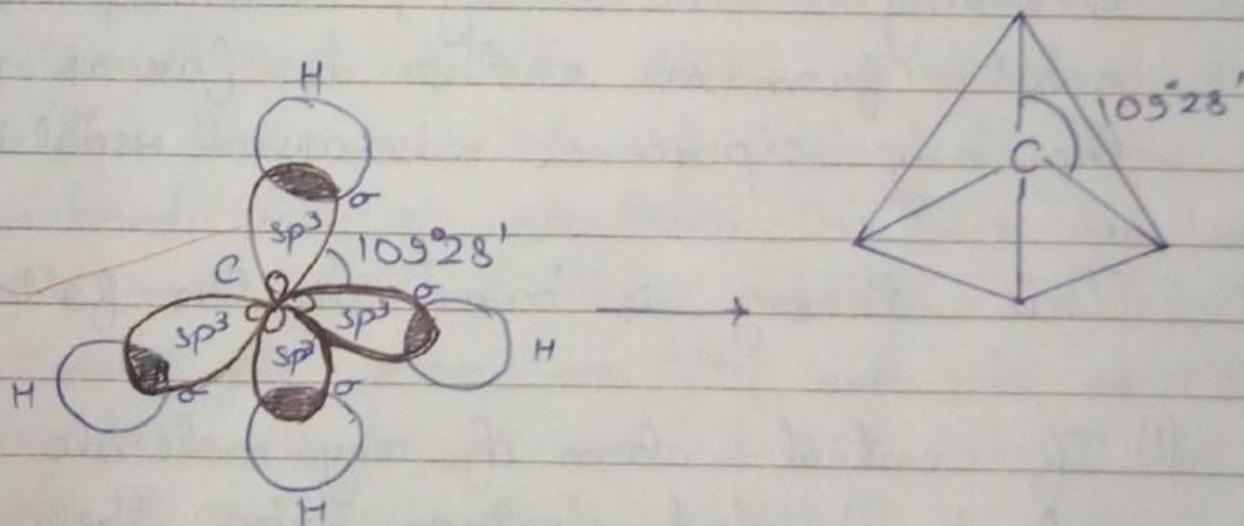
These four orbitals are directed towards a regular tetrahedron as in this state repulsion between them becomes minimum. Molecule containing such a sp^3 -hybrid central atom are of tetrahedral shape. Here the central atom is carbon. This hybridisation is also called tetrahedral hybridisation.



Example →

(i) Formation of Methane (CH_4) —

Configuration of carbon atom ~~in its~~ excited state is $1s^2, 2s^1, 2p_x^1, 2p_y^1, 2p_z^1$. One 2s and three p (p_x, p_y and p_z) orbitals together form four sp^3 -hybrid orbitals, which make an angle of $105^\circ 28'$ among themselves. Such carbon atom form four sp^3 -s sigma bonds with four H atoms and methane molecule attains a tetrahedral structure.



Valence Shell Electron Pair Repulsion Theory or VSEPR Theory

It has been observed that structure of many covalent molecules cannot be explained only on the basis of hybridisation. Sidgwick and Powell in 1940 proposed valence shell electron pair repulsion (VSEPR) theory to explain the shape of polyatomic molecules.

According to this theory, shape of a polyatomic molecule depends upon the arrangement of covalent bonds formed by the central atom and this arrangement depends upon the shape and size of electron pairs and orbitals of valence shell.

According to this theory, electron pairs tend to keep apart from one another as far as possible so that they may experience minimum repulsive interaction.

This theory is based on the following points:

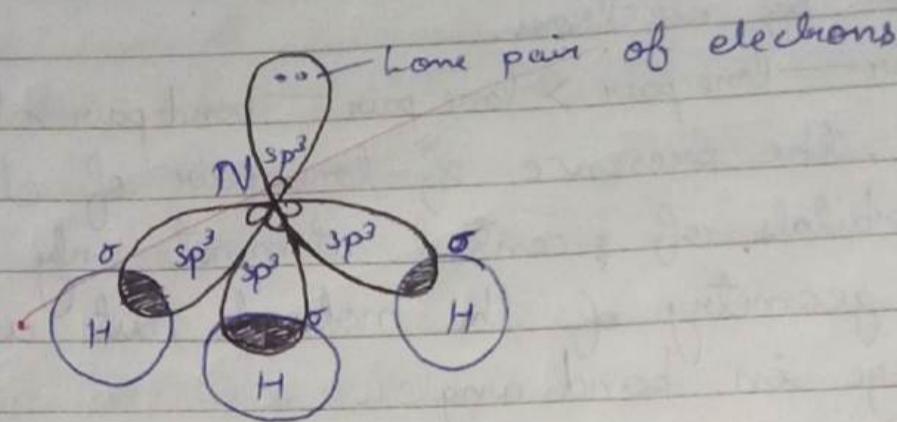
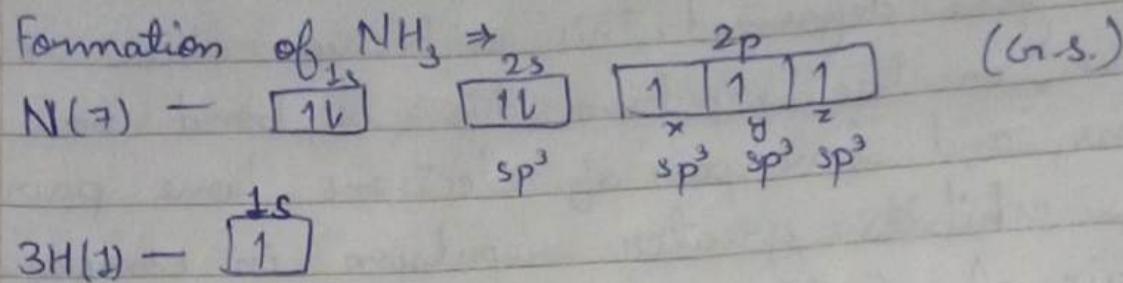
- (1) If central atom of any molecule is surrounded only by bonded electron pairs then shape of the molecule is symmetrical and depends on the number of bonded electron pairs.
Ex: BeCl_2 , CO_2 etc.
- (2) When the hybrid orbital of the central atom of a molecule possesses a lone pair of electrons along with bond pair of electrons the regular shape of the

molecule gets deformed. This is because there is a difference in the repulsion due to bond pair of electrons and lone pair of electrons. Lone pair of electrons exhibits greater repulsion in comparison to bond pair of electrons.

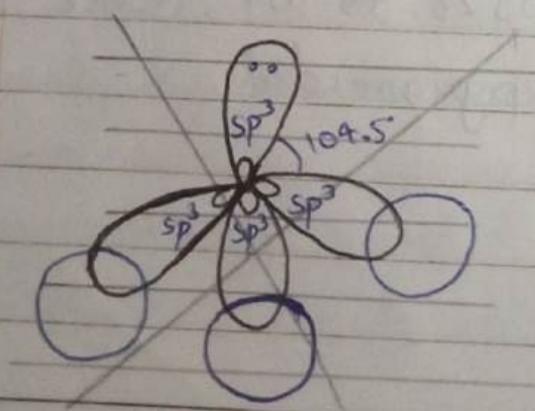
lone-pair — lone-pair > lone-pair — bond-pair > bond-pair — bond-pair
 Therefore, the presence of lone-pair of electrons in the hybrid orbitals of central atom not only deforms the regular geometry of the molecule, but also brings about a change in bond angle.

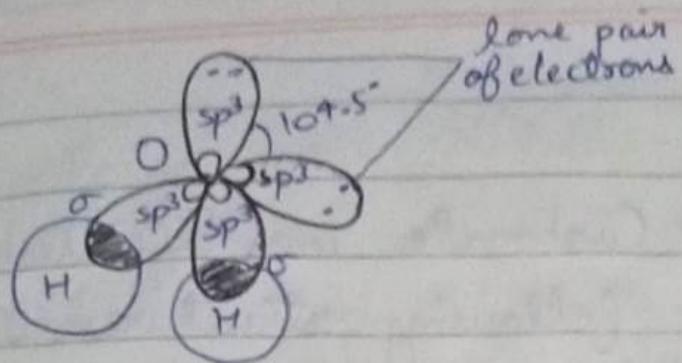
For example →

- (1) Shape of NH_3 molecule → sp^3 -hybridisation is assumed in the central nitrogen atom of the ammonia molecule.
 Its four sp^3 -hybrid orbitals have regular tetrahedral geometry. One of the sp^3 hybrid orbital has one lone pair of electrons. Rest of the three sp^3 -hybrid orbitals overlap with the s-orbitals of hydrogen atoms to have three bond pair of electrons. One lone-pair of electrons has more repulsion than bond-pair of electrons. Therefore, hence, the shape of NH_3 molecule is H-N-H bond angle decreases from $109^\circ 28'$ to 107° . Hence, the shape of NH_3 molecule is trigonal pyramidal.



(ii) Shape of H_2O molecule \rightarrow sp^3 -hybridisation is found in the central oxygen atom of H_2O . Hence, it should have regular tetrahedral structure. And among four sp^3 -hybrid orbitals obtained by sp^3 -hybridisation, two have lone-pair of electrons. Rest of the two sp^3 -hybrid orbitals overlap with the s-orbital of hydrogen atoms to have bond-pair of electrons. Due to higher repulsion of two lone-pair of electrons bond angle reduces from $109^\circ 28'$ to ~~$104^\circ 5'$~~ 104.5° . Regular tetrahedral geometry get deformed to angular or bent or V shape.





Resonance

Structure of a molecule is decided by chemical bonding. This structure explains all the properties of a compound. When the molecular structure of a compound is unable to explain all of its properties then its other structures are assumed. If none of these structures can exactly describe all the properties of the compound then the structure explaining all of its properties is called resonance hybrid.

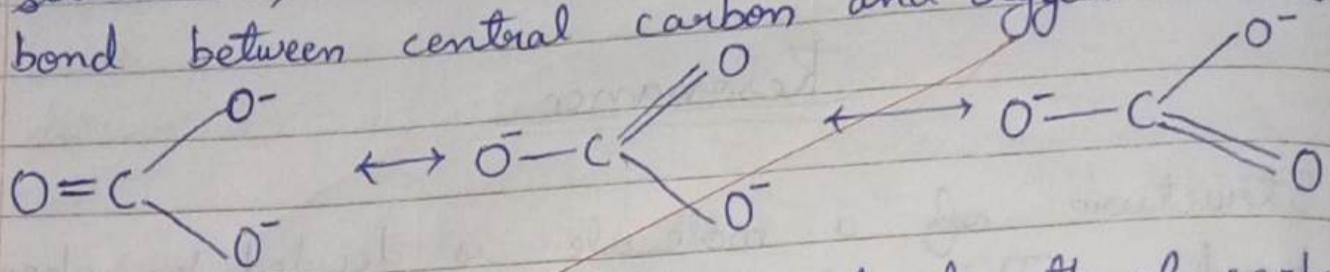
This phenomenon of the compound is called resonance.

Characteristics of Resonance

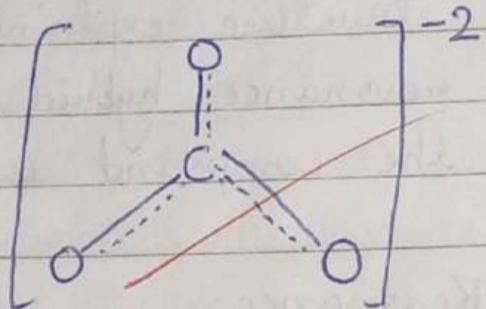
- 1) Actual structure of a molecule which is called resonance hybrid is unknown but in fact it has its existence.
- 2) It is not possible to exhibit the actual structure of the structure of resonance hybrid of a molecule.
- 3) Canonical forms of a molecule are imaginary.
- 4) A molecule attains stability due to resonance.

Example -

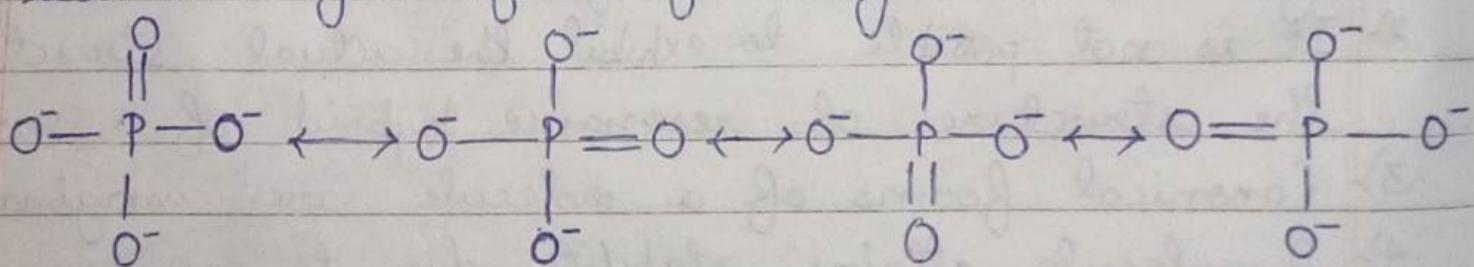
Carbonate ion (CO_3^{2-}) \rightarrow Carbonate ions (CO_3^{2-}) is a resonance hybrid of the following structures. In these structures, there are two single bonds and one double bond between central carbon and oxygen atoms.



In this ion, experimental bond length of carbon-oxygen bond is 1.31 \AA , which is average of calculated values of bond length of $\text{C}=\text{O}$ (1.22 \AA) and $\text{C}-\text{O}$ (1.43 \AA) bonds. For convenience resonance hybrids can be represented in the following way:



Phosphate ion (PO_4^{3-}) \rightarrow Phosphate ion (PO_4^{3-}) is a resonance hybrid of the following resonance structures:



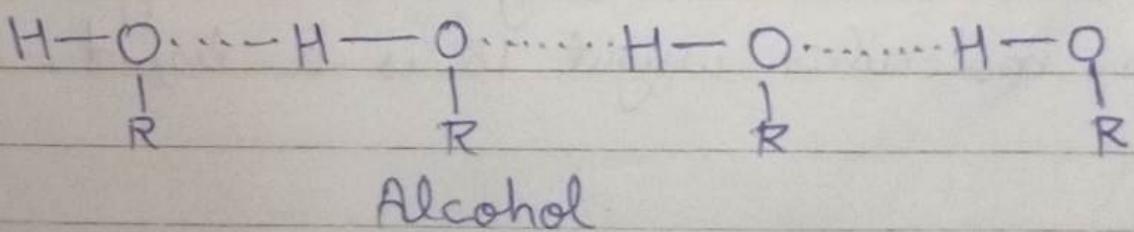
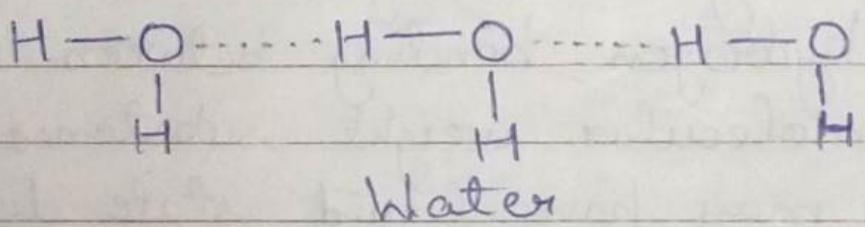
Hydrogen Bond

When hydrogen atom is attached to a strongly electronegative atom, like - oxygen (O), nitrogen (N) or fluorine (F) etc., through a covalent bond, then shared electron pair shifts towards the more electronegative atom. As a result, the hydrogen atom becomes electropositive with respect to the other atom. This hydrogen develops a capacity to form a bond with another electronegative atom. Such a bond is called hydrogen bond. It is represented by a dotted line (...) whereas a covalent bond is represented by a dash. It acts as a bridge between two covalent bonds hence, hydrogen bond is also called hydrogen bridging.

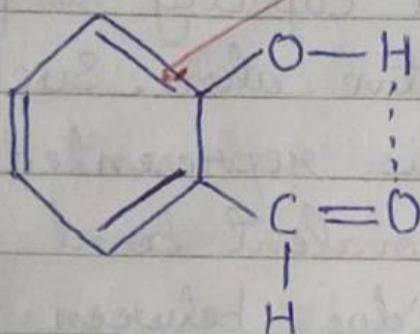
Types of Hydrogen Bonds

- Intermolecular hydrogen bond → This hydrogen bond is formed between two molecules. In this several molecules get associated by a hydrogen bond. This is also called association.

Example →



2) Intramolecular hydrogen bond \rightarrow When hydrogen bond is formed between H atom and other atom of the same molecule then it is called intramolecular hydrogen bonding or chelation. Both types of hydrogen bonding affect the properties of compounds in different ways. Like,



$\text{o-Hydroxy benzaldehyde}$

Influence of Hydrogen Bonding on the Properties of Compounds

(1) Physical state of matter — According to kinetic theory of matter if the substance of high molecular weight is a gas then the molecules of the low molecular weight substance being far apart from each other would definitely be in gaseous state. Now if there is hydrogen bonding between the molecules of low molecular weight substance then the substance may have liquid state due to the decrease in intermolecular distance. For example, H_2S with molecular weight 34 is a gas whereas H_2O with molecular weight 18 is a liquid.

- 2) Boiling and melting points — Normally, boiling and melting points of compounds of elements in one group increase with increasing molecular mass, but boiling and melting points of H_2O , NH_3 and HF are more than H_2S , PH_3 and HCl . The reason is that molecules of compounds H_2O , NH_3 and HF are attached with other molecules through hydrogen bonding, i.e., are associated. Extra heat is required to break these intermolecular hydrogen bonds, due to which their boiling and melting points become high.
- 3) Ice is lighter than water — Water molecule is bonded to four other water molecules in solid state. As a result, molecule of water has a tetrahedral structure. There is a plenty of space between the tetrahedral lattices because of which density of ice is less than of water and ice is lighter ~~than~~ than water and floats on it.
- 4) Water contracts between $0^\circ C$ and $4^\circ C \rightarrow$ Water has maximum density at $4^\circ C$. When water is heated it contract first. When it is heated from $0^\circ C$ to $4^\circ C$ then hydrogen bonds present in water start breaking as a result, molecules of water come close to each other. Thus, water contracts and its density also increases. Above $4^\circ C$ expansion dominates hence water molecules move away from each other.

- 5) Solubility → Alcohol and carboxylic acid dissolve in water since they form hydrogen bonds with molecules of water. In this way, many organic compounds dissolve in water. Alkane and alkenes do not form hydrogen bonds with water and hence are insoluble.
- 6) High viscosity, high heat of vaporisation and high dielectric constant → Due to hydrogen bond, viscosity of glycerol ($\text{CH}_2\text{OH}-\text{CHOH}-\text{CH}_2\text{OH}$) is more as compared to water and ~~old~~ alcohol. Due to large amount association large amount of heat is required for its vaporisation. Therefore, it has high heat of vaporisation.

1st term course completed.