## UNIT 4 - CHEMICAL BONDING AND MOLECULAR STRUCTURE

## Concept -VSEPR \& VBT

## KNOWLEDGE

## One Mark Questions

Q1. On the basis of VSEPR theory predict the shape of Hydronium $\left(\mathrm{H}_{3} \mathrm{O}^{+}\right)$ion (L-1)
Ans. pyramidal.

Q2 what is the electrovalency of Li and O in $\mathrm{Li}_{2} \mathrm{O}$ compound?(L-1)
Ans. Electrovalency of each Li atom is one while that of oxygen atom is 2.

Q3. What is the value of 1 Debye unit?(L-1)
Ans. $1 \mathrm{D}=3.33564 \times 10^{-30} \mathrm{C}$ _m

Q4.Define formal charge of an atom. (L-1)
Ans.The formal charge is the difference between the number of valence electrons in an isolated atom and the number of electrons assigned to that atom in a LEWIS STRUCTURE

Q5.Which rule explains the covalent character of ionic bond ?(L-1)
Ans. Fajan's Rule

## Two Marks Questions

Q1.Define Bond length\& Bond dissociation enthalpy(L-1).
Ans. The equilibrium distance between the centre $s$ of the nuclei of two bonded atoms is called bond length.
The energy required to break a bond is called bond dissociation enthalpy.

Q 2. Give Four examples of molecules showing extended octet rule.(I-1)
Ans. $\mathrm{PCl}_{5}, \mathrm{SF}_{6}, \mathrm{IF}_{7}, \mathrm{SF}_{4}$

Q 3.On the basis of VSEPR theory give the geometry \& bond angle of (I-2)
(i) $\mathrm{BF}_{3}$
(ii) $\mathrm{SiH}_{4}$

Ans. Trigonal planar $120^{\circ}$
Tetrahedral $109.5^{\circ}$

Q 4.What is the geometry of molecule of type $\mathrm{AB}_{4} \mathrm{E}_{2}$ \& $\mathrm{AB}_{3} \mathrm{E}(\mathrm{L}-2)$
Ans. Square planar \& Pyramidal shape

Q 5. Write two limitation of VSEPR theory(L-1).
Ans. (i) It is unable to predict the shapes of many molecules
(ii) It does not consider the directional effect of bonding.

## Three Marks Questions

Q 1.What is the expended octet? Write any three example of compound showing expended octet ? (L-1)

Ans. Elements in and beyond third period of periodic table have, apart from $3 \mathrm{~s} \& 3 \mathrm{p}$ orbital ,3d orbital also available for bonding. In a number of compounds of this elements there are more than 8 valence electron around central atom. This is termed as expended octet.

Ex. $\mathrm{PF}_{5}, \mathrm{SF}_{6}, \mathrm{H}_{2} \mathrm{SO}_{4}$

Q 2.(a)State one significance of Formal Charge.(L-2)
Answer. It helps us to select the most stable structure out of all the different Lewis structures.
(b)In nitrate ion what should be total of Formal Charge on each atom? Why?

Ans. The sum of formal charge is always equal to the charge present on the ion. Hence sum of charges in $\mathrm{NO}_{3}^{-}$will be -1.

Q3. On the basis of VSEPR THEORY \& VBT THEORY answer the following-(L-3)
a) What is the Shape of $\mathrm{SF}_{4}$ ?

b) NaCl gives a white ppt. with $\mathrm{AgNO}_{3}$ but $\mathrm{CCl}_{4}$ does not. Why?.

Answer. Being an ionic compound NaCl gives Cl negative ion and thus gives White ppt. with silver nitrate but $\mathrm{CCl}_{4}$ is a covalent compound and thus do not give Cl negative ions.
c) Calculate sigma and pi bond-


Ans. 5 sigma and 1 pie bond

Q4.Dipole moment of $\mathrm{NH}_{3}$ is greater than of $\mathrm{NF}_{3}$.?(L-3)
Ans. Resultant moment of N-H bond adds up to the bond moment of lone pair, that of $3 \mathrm{~N}-\mathrm{F}$ bonds partly cancels the resultant moment of lone pair. Thus the dipole moment of $\mathrm{NH}_{3}$ is greater than of $\mathrm{NF}_{3}$.
5.Name factors which are responsible for covalent character of ionic bond(I-1).
(i) Large size of anion
(ii) Small size of cation
(iii) Electronic configuration of the cation

## UNDERSTANDING

## One Mark Question

Q1. Explain why $\mathrm{PCl}_{5}$ is trigonal bipyramidal and $\mathrm{IF}_{5}$ is square pyramidal?(L-2)
Ans. $\mathrm{PCl}_{5}$ has 5 bond pairs of electrons around central atom while in $\mathrm{IF}_{5}$ there are 5 bond pair \& 1 lone pair of electrons around central atom.
Q2.Arrange the following in the order of decreasing bond angle.(L-2)

$$
\mathrm{NO}_{2}^{+}, \mathrm{NO}_{2}^{-}, \mathrm{NO}_{2}
$$

Ans. $\mathrm{NO}_{2}^{+}>\mathrm{NO}_{2}>\mathrm{NO}_{2}{ }^{-}$

Q3.Why are tripositive and tetrapositive cations rare ? $\mathrm{LI}-2$ )
Ans. Highly charged cations such as $3^{+}$and $4^{+}$ions are formed by the removal of 3 and 4 erespectively from the neutral atoms. For this purpose, a large amount of energy( $E_{1}+E_{2}+E_{3} O R$ $\left.E_{1}+E_{2}+E_{3}+E_{4}\right)$ is required.

Q 4. Why does H2O molecule have bent geometry Bent geometry?(L-2)
Ans. Due to repulsion $b / n$ two lone paires of e-present around central atom 0

Q 5..What is the cause of chemical combinationl(L-1)
Ans. The tendency of atoms of various elements to acquire stable configuration of the nearest noble gas is the cause of chemical combination.

## Two Marks Questions

Q 1.Give Reason(L-2)
(i) $\mathrm{N}_{2}$ is inert at room temperature.
(ii) Overlapping of $S$ orbital with any other orbital forms sigma bonds.

Ans .Due to high bond order (3) , it has high bond dissociation energy, which is not possible at room temperature
(ii)Because s orbital has same electron distribution in all axis/ directions

Q 2 .What is bond enthalpy ? What is its unit ? How we calculate enthalpy in case of complex compound ?(L-2)
Ans. Amount of energy Required ot break one mole of bonds of particular type $b / w$ two atoms in gaseous state.
Its unit is $\mathrm{KJ} /$ mole
It is obtained by dividing total bond dissociation enthalpy by no. of bonds broken

Q 3 .How does covalent bond form in terms of orbital overlap concept?(L-1)
Ans. When two half filled orbitals overlap ,covalent bond forms .

## Q 4.Out of $\mathrm{NH}_{3} \& \mathrm{BF}_{3}$ Which is polar \& Why?(L-2)

Ans. $\mathrm{NH}_{3}$ has net dipole moment because resultant of $3 \mathrm{~N}-\mathrm{H}$ bond \& lone pair lie in the same direction. While BF3 being trigonal planar has zero dipole moment.

Q 5.When does ionic character develop in covalent bond?(L-3)
Ans. When the difference in electro negativity of the combining atom is more than 1.9 it develops 50 \% ionic character .

## Three Marks Questions

Q 1.Molecule has a type $A B_{3} E_{2}$. Draw its structure and state an example.(L-3)


The $\mathrm{F}-\mathrm{Cl}-\mathrm{F}$ angle involving the axial $F$ atoms is $175^{\circ}$


The red lines outline a trigonal bipyramid. Black lines show the electron pairs
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Q 2.Draw the potential energy curve Of $\mathrm{H}_{2}$ molecule formation?(L-3)


Q 3 .Account for the following :(L-3)
(i) $\mathrm{AlF}_{3}$ is a high melting point solid whereas $\mathrm{SiF}_{4}$ is a gas?

Ans. $\mathrm{AlF}_{3}$ is an ionic solid due to large difference in electro negativity of Al and F whereas $\mathrm{SiF}_{4}$ is a covalent compound and hence only weak Vander Waals force exists between the molecules.
(ii) Out of peroxide ion and superoxide ion which has larger bond length and why?

Ans. The bond orders of(superoxide ion) $\mathrm{O}_{2}{ }^{-}$is 1.5 while that of(peroxide ion ) $\mathrm{O}_{2}{ }^{2-}$ is 1.0 .Smaller the bond order, greater the bond length. Hence, $\mathrm{O}_{2}{ }^{2-}$ has larger bond length.

Q4. What do you mean by canonical structures? Draw canonical structures of Carbonate ion \& Benzene. [1+2](L-3)
Ans. Sometimes a molecule possess several structures and the actual one is in between of them. This is called Canonical structure.



Q5. Draw the structures of $\mathrm{H}_{2} \mathrm{SO}_{4}, \mathrm{H}_{3} \mathrm{PO}_{4} \cdot[2+1=3](\mathrm{L}-2)$
Answer.



## APPLICATION

## One Mark Questions

Q 1.Define polarizing power and polalrisability(L-2)
Ans. The ability of an atom to deform the electron cloud of an atom is called polarizing power . while the ease with which any atom can be polarized by its neighbouring bonded atom is called polarizability.

Q 2.Why $\mathrm{PCl}_{5}$ is more covalent than $\mathrm{PCl}_{3}$ ? (L-2)
Ans. Because $\mathrm{P}^{5+}$ has more polarising power than $\mathrm{P}^{3+}$.

Q 3.Draw Resonating structure of $\mathrm{O}_{3}$.(L-3)

$$
0-0-0
$$

Add 1 double bond and unshared electron pairs so that each element will have an octet of electrons around it


Two equivalent resonance forms for $\mathrm{O}_{3}$

Q 4. Why is $\mathrm{SF}_{4}$ more reactive than $\mathrm{SF}_{6}$ ?(L-2)
Ans. $\mathrm{SF}_{4}$ has two unpaired electrons which it can donate further to extend its valency, hence it is reactive .'S' in $\mathrm{SF}_{6}$ has maximum 6 0.S.

Q 5.Explain the following order of bond angle (L-2)

$$
\mathrm{NO}_{2}^{+}>\mathrm{NO}_{2}>\mathrm{NO}_{2}^{-}
$$

Ans. This is because $\mathrm{NO}_{2}{ }^{+}$has no lone pair of e-, and hence its linear. $\mathrm{NO}_{2}$ has one unshared e- while $\mathrm{NO}_{2}$ has one unshared e- pair. Greater the repulsion on $\mathrm{N}-\mathrm{O}$ bond in case of $\mathrm{NO}_{2}{ }^{-}$than in case of $\mathrm{NO}_{2}$.

## Two Marks Questions

Q 1.Suggest the expected shape of the following molecules with reasons(L-2)
a. $\mathrm{SO}_{2}$
b. $\mathrm{NH}_{3}$

Ans.(a) In $\mathrm{SO}_{2}$ molecule there are three electron pairs .the three electron pairs should acquire trigonal planar arrangement with bond angle $120^{\circ}$. Since one of the position is occupied by lone pair the geometry is described as V-shaped or bent shaped.
(b) In $\mathrm{NH}_{3}$ molecule there are are four electron pairs (three bond pairs and one lone pair). These four electron pairs adopt tetrahedral geometry but due to the repulsion by lone pair the bond decreases to $107^{\circ}$ from $109.5^{\circ}$ and hence the geometry of ammonia is regarded as pryamidal.

Q 2. Why is $\mathrm{CO}_{2}$ a linear molecule while $\mathrm{SO}_{2}$ a non-linear molecule?(L-2)
Ans. In $\mathrm{SO}_{2}$ molecule there are two bond pairs and one lone pair of electron .Due to repulsion by lone pair its bond angle decreases from $120^{\circ}$ to $119.5^{\circ}$ hence it is not linear whereas in $\mathrm{CO}_{2}$ molecule there is no lone pair of electron due to which it has linear geometry.

Q 3. Why $\mathrm{He}_{2}$ molecule does not exist?(L-2)
Ans. It has been found that when two helium atoms approach each other four new attractive forces and five new repulsive forces come into play. Therefore repulsive forces predominate and the potential energy of the system increases which leads to instability. Or Bond order is Zero.

Q 4. Apart from tertrahedral geometry, another possible geometry for $\mathrm{CH}_{4}$ is square planar with the four H atoms at the corners of square and C atom at its centre. Explain why $\mathrm{CH}_{4}$ is not square planar.(L-3)
Ans. In square planar geometry, the bond angle will be $90^{\circ}$ which is less than bond angle in tetrahedral geometry ( $109.5^{\circ}$ ).Therefore repulsive forces in square planar will be more and it will be less stable as compared to tetrahedral geometry.

Q 5.Explain the formation of $\mathrm{H}_{2}$ molecule on the basis of valence bond theory.(L-2)
Ans. When two H atoms come closer the following forces operate between them:
a. Attractive :
i.nucleus of atom and its electron
ii.nucleus of one atom and electron of other.
b.repulsive :
i.electrons of two atoms.
ii.nucleus of two atoms.

It has been found experimentally that magnitude of attractive forces is more than repulsive forces hence two atoms come closer to each other and the potential energy of the system decreases. A stage is reached when attractive forces balance repulsive forces and the system acquires minimum energy .At this stage two hydrogen atoms are said to be bonded together.

## Three Marks Questions

Q1. i) Write Lewis dot structure for HCOOH . (L-2)
ii)Ethyne molecule is linear.

Ans: i)

(ii)Ethyne has 'sp' hybridisation and thus is linear in shape.

Q2. i) Calculate formal charges of the atoms in nitrite ion.(L-2)
Ans. i) Formal charge $=\mathrm{V}-\mathrm{L}-1 / 2 \mathrm{~S}$
V--Total no. of valence electrons in free atom
L-- Total no.of non-bonding electrons
S-- $1 / 2$ Total no. of bonding electrons
(ii)


For $N=5-2-1 / 26=5-3=0$
For $\mathrm{O}=6-4-1 / 24=2-2=0$
For $O(-$ vely charged) $=6-6-1 / 2 \times 2=-1$
Total charge = -1

Q 3 structures for $\mathrm{H}_{2} \mathrm{CO}_{3}, \mathrm{SF}_{6}$, PF5 and $\mathrm{IF}_{7}$. Is the octet rule obeyed in all these cases?

Ans. (i) $\mathrm{H}_{2} \mathrm{CO}_{3}$
(ii) $\mathrm{SF}_{6}$


12 electrons around the $S$ atom
(iii) $\mathrm{PF}_{\mathbf{s}}$


10 electrons around the $P$ atom
(iv) $\mathrm{IF}_{7}$


H -atom has two valence electrons. $C$ and three $O$ atoms obeying octet rule.

S-atom has 12 valence electrons. S-atom is not obeying octet rule.

There are 10 electrons around the $\mathbf{P}$ atom. $\mathbf{P}$ has an expanded octet.

I is not obeying the octet rule.

Q3. i) Why is bond angle in $\mathrm{PH}_{4}{ }^{+}$higher than that in $\mathrm{PH}_{3}$ ? (L-2)
Ans : P in $\mathrm{PH}_{3}$ is $s p^{3}$ hybridized. $\mathrm{PH}_{3}$ has three bond pairs and one lone pair around P . Due to stronger lone pair-bond pair repulsions than bond pair-bond pair replulsions, the tetrahedral angle decreases from $109.5^{\circ}$ to $93.3^{\circ}$. As a result, $\mathrm{PH}_{3}$ is pyramidal. However, when it reacts with a proton, it forms $\mathrm{PH}_{4}{ }^{+}$ion which has four bond pairs and no lone pair. Due to the absence of lone pair-bond pair repulsions and presence of four identical bond pair-bond pair interactions, $\mathrm{PH}_{4}{ }^{+}$ assumes tetrahedral geometry with bond angle of $109.5^{\circ}$. This explains why the bond angle in $\mathrm{PH}_{4}{ }^{+}$is higher than in $\mathrm{PH}_{3}$. (See Fig. 32.3)


(Tetrahedradal)

Fig 32.3 Bond angle in $\mathrm{PH}_{4}{ }^{+}$is larger than that in $\mathrm{PH}_{3}$.
ii) Arrange the bonds in order of increasing ionic character in the molecules: (L3) $\mathrm{LiF}, \mathrm{K}_{2} \mathrm{O}, \mathrm{N}_{2}, \mathrm{SO}_{2}$ and $\mathrm{ClF}_{3}$.
Ans- $\mathrm{N}_{2}<\mathrm{SO}_{2}<\mathrm{ClF}_{3}<\mathrm{K}_{2} \mathrm{O}<\mathrm{LiF}$.

Q4. i) Explain why BeH 2 molecule has a zero dipole moment although the $\mathrm{Be}-\mathrm{H}$ bonds are polar.(L-2)

Ans. The Lewis structure for BeH 2 is as follows:


There is no lone pair at the central atom ( Be ) and there are two bond pair. It has a linear structure. Dipole moments of each $\mathrm{H}-\mathrm{Be}$ bond are equal and are in opposite directions. Therefore, they nullify each other and the $\mathrm{BeH}_{2}$ molecule has zero dipole moment.
ii) Although both $\mathrm{CO}_{2}$ and $\mathrm{H}_{2} \mathrm{O}$ are triatomic molecules, the shape of $\mathrm{H}_{2} \mathrm{O}$ molecule is bent while that of $\mathrm{CO}_{2}$ is linear. Explain this on the basis of dipole moment.
Ans. $\mathrm{CO}_{2}$ molecule has only two bonds which lie farthest to each other to minimise repulsion, making an angle of $180^{\circ}$.


$\mathrm{H}_{2} \mathrm{O}$, on the other hand, has a lone pair. As lone pair- bond pair repulsion is greater than bond pairbond pair repulsion, the repulsions due to the lone pair decreases the angle between the two bonds, giving the molecule a bent shape.

Q5. Describe the shape of $\mathrm{PCl}_{5}$ molecule. Why are the axial bonds longer as compared to equatorial bonds?(L-3)
Ans: The ground state and excited state outer electronic configurations of phosphorus $(Z=15)$ are: Excited state:
$\mathrm{Ne} 3 \mathrm{~s}^{1} 3 p_{\mathrm{x}}{ }^{1} 3 \mathrm{p}_{\mathrm{y}}{ }^{1} 3 \mathrm{p}_{\mathrm{z}}{ }^{1} 3 \mathrm{~d}^{1}$
Phosphorus atom is $s p^{3} d$ hybridized in the excited state. These orbitals are filled by the electron pairs donated by five Cl atoms.
The five $s p^{3} d$ hybrid orbitals are directed towards the five corners of the trigonal bi-pyramidals. Hence, the geometry of PCI5 can be represented as:


There are five $\mathrm{P}-\mathrm{Cl}$ sigma bonds in $\mathrm{PC}_{15}$. Three $\mathrm{P}-\mathrm{Cl}$ bonds lie in one plane and make an angle of $120^{\circ}$ with each other. These bonds are called equatorial bonds. The remaining two $\mathrm{P}-\mathrm{Cl}$ bonds lie above and below the equatorial plane and make an angle of $90^{\circ}$ with the plane. These bonds are called axial bonds. As the axial bond pairs suffer more repulsion from the equatorial bond pairs, axial bonds are slightly longer than equatorial bonds

## Concept- Hybridisation and Molecular Orbital Theory

## KNOWLEDGE

## One mark questions

Q1 Who gave MOT (L-I)
Ans Molecular orbital (MO) theory was developed by F. Hund and R.S. Mulliken in 1932

Q2 Write the shape and bond angle of $s p$ hybrid orbitals? (L-II)
Ans Linear, $180^{\circ}$

Q3 What is the state of hybridization of carbon atom in (i)diamond (ii) Graphite (L-III) Ans. $s p^{3}, \mathrm{sp}^{2}$

Q4 What is the shape and hybridization of $\mathrm{NH}_{4}{ }^{+}$ion ? (L-II)
Ans $\mathrm{sp}^{3}$ tetrahedral

Q5 Write the shape and bond angle of $\mathrm{sp}^{2}$ hybridized orbitals.(L-II)
Ans. Trigonal planar and bond angle $120^{\circ}$
Two marks questions
Q1 What is hybridization? (L-I)
Ans: The process of intermixing of atomic orbitals of slightly different energies of same atom to get same number of new orbitals of equivalent energies and shape is called hybridization

Q2 Which hybrid orbital are used by carbon atoms in the following molecules (L-II)
(a) $\mathrm{CH}_{3} \mathrm{CH}_{2} \mathrm{OH}$
b) $\mathrm{CH}_{3} \mathrm{COOH}$.
Ans a) $\mathrm{sp}^{3}, \mathrm{sp}^{3}$
b) $\mathrm{sp}^{3} \mathrm{sp}^{2}$

Q3. Give an example for $\mathrm{sp}^{2}$ and $\mathrm{sp}^{3}$ hybrid molecules also give their shape (L-II)
Ans $\mathrm{sp}^{2}$-Trigonal planar e.g, $\mathrm{BH}_{3}$
sp ${ }^{3}$ - Tetrahadral eg $\mathrm{CH}_{4}$
Q4 . Draw the shapes of following hybrid orbitals. $s p, p^{2}$ (L_II)

Ans sp B_A_B


Q5. Draw the shapes of $\mathrm{H}_{2} \mathrm{O}$ and $\mathrm{CH}_{4}$ molecule (L-II)
Ans

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## Three Marks Questions

Q1 Give conditions for the combination of Atomic Orbitals (L-I)
Ans i).The combining atomic orbitals must have the same or nearly the same energy
ii). The combining atomic orbitals must have the same symmetry about the molecular axis
iii) The combining atomic orbitals must overlap to the maximum extent

Q2 Explain the formation of $\mathrm{BCl}_{3}$ using hybridization (L-II)
Ans $\ln \mathrm{BCl}_{3}$ molecule, the ground state electronic configuration of central boron atom is $1 s^{2} 2 s^{2} 2 p^{1}$. In the excited state, one of the $2 s$ electrons is promoted to vacant $2 p$ orbital as


Q3 Give important conditions for Hybridisation. Give Hybridisation and shape of $\mathrm{IF}_{7}$ (L-I)
Ans Important conditions for hybridisation
(i) The orbitals present in the valence shell of the atom will take part in hybridisation.
(ii) The orbitals undergoing hybridisation should have almost equal energy
(iii) Promotion of electron is not essential condition prior to hybridisation.
(iv) It is not necessary that only half filled orbitals participate in hybridisation. In some cases, even filled orbitals of valence shell take part in hybridisation.
$\mathrm{sp}^{3} \mathrm{~d}^{3}$ and pentagonal bipyramidal.

Q4 Give salient features of Molecular orbital theory (L-I)
Ans (i) The electrons in a molecule are present in the various molecular orbitals as the electrons of atoms are present in the various atomic orbitals.
(ii) The atomic orbitals of comparable energies and proper symmetry combine to form molecular orbitals.
(iii) In a molecular orbital an electron is influenced by two or more nuclei depending upon the number of atoms in the molecule.
(iv) The number of molecular orbital formed is equal to the number of combining atomic orbitals. When two atomic orbitals combine, two molecular orbitals are formed. One is known as bonding molecular orbital while the other is called antibonding molecular orbital.
(v)The bonding molecular orbital has lower energy and hence greater stability than the corresponding antibonding molecular orbital.
(vi) The electron probability distribution around a group of nuclei in a molecule is given by a molecular orbital.
(vii) The molecular orbitals like atomic orbitals are filled in accordance with the aufbau principle obeying the Pauli's exclusion principle and the Hund's rule.

Q5 What is the hybrid state of $\mathrm{BeCl}_{2}$. What will be the change in hybrid state of $\mathrm{BeCl}_{2}$ in solid state?(L-II)

Ans. In vapour state $\mathrm{BeCl}_{2}$ is linear with sp hybridization .In solid state it has polymeric chain with chlorine bridges Two Cl atom are linked to Be atom by coordinate bond and two by covalent bond .For these bonds to be in excited state with configuration $1 s^{2} 2 s^{1} 2 p_{x}{ }^{1} 2 p_{y}{ }^{0} 2 p_{z}^{0}$ undergoes $s p^{3}$ hybridisation Two half filled hybrid orbitals will form covalent bond with two Cl atoms The other two Cl atoms are coordinated to Be atom by donating electron pairs into empty hybrid orbitals


## UNDERSTANDING

## One mark questions

Q1 Arrange the following orbitals in the increasing order of $s$ - character: $s p, p^{2}, \mathrm{sp}^{3}(\mathrm{~L}-\mathrm{I})$
Ans. $\mathrm{sp}^{3}<\mathrm{sp}^{2}<\mathrm{sp}$

Q2 How is paramagnetic character of a compound is related to the no. of unpaired electrons?(L-II) Ans. Greater the number of unpaired electrons greater will be the paramagnetic character

Q3. Calculate bond order of $\mathrm{N}_{2}$ ? (L-II)
Ans. 3

Q4 Give electronic configuration for $\mathrm{C}_{2}$ ? (L-1)
Ans. $\sigma_{1 \mathrm{~s}}{ }^{2} \sigma^{*}{ }_{1 \mathrm{~s}}{ }^{2} \sigma_{2 \mathrm{~s}}{ }^{2} \sigma^{*}{ }_{2 \mathrm{~s}}{ }^{2} \pi_{2 \mathrm{py}}{ }^{2} \pi_{2 \mathrm{pz}}{ }^{2}$

Q5 Calculate the number of unpaired electrons in the $B_{2}$ molecule (L-I)
Ans 2

## Two marks questions

Q1 Considering $X$ - axis as the internuclear axis, which out of the following will not form sigma bond?
Why? a) 1 s and 2 s b) 1 s and 2 px c) 2 py and 2 py d) 1 s and 2 s (L-III)
Ans (c) since overlapping of $p$ orbitals side wise results in formation of pi bond and $x$ axis is being considered as internuclear axis

Q2 Distinguish between bonding molecular orbital and anti-bonding molecular orbital.(L-II)
Ans.(i)The bonding molecular orbital has lower energy and hence greater stability than the corresponding antibonding molecular orbital.
(ii) Just as the electron probability distribution around a nucleus in an atom is given by an atomic orbital, the electron probability distribution around a group of nuclei in a molecule is given by a molecular orbital.
(iii)The molecular orbital formed by the addition of wave functions of atomic orbitals is called the bonding molecular orbital while the molecular orbital formed by the subtraction of wave function of atomic orbital is called antibonding molecular orbital

Q3 Define bond order and give the relationship between bond order and bond length (L-I) Ans Bond order (b.o.) is defined as one half the difference between the number of electrons present in the bonding and the antibonding orbitals i.e., Bond order (b.o.) $=1 / 2(\mathrm{Nb}-\mathrm{Na})$ Bond order is inversely proportional to bond length

Q4 Apart from tetrahedral geometry another possible geometry for $\mathrm{CH}_{4}$ is square planar with four hydrogen atoms at the corners of the square and the carbon atom at the centre.Explain why $\mathrm{CH}_{4}$ is not square planar? (L-II)
Ans For square planar arrangement hybridization is $\mathrm{dsp}^{2}$ which is not possible with Carbon as it does not have d orbital with it

Q5 Out of p-orbital and sp hybrid orbital which has greater directional character and why ? (L-III) Ans $s p$ because lobes of $p$ orbital have equal electron density whereas $s p$ hybrid orbital has greater electron density on one side

## Three Marks Questions

Q1Explain the formation of $S F_{6}$ using $s p^{3} d^{2}$ hybridization (L-I)


Ans. In $\mathrm{SF}_{6}$ the central sulphur atom has the ground state outer electronic configuration $3 s^{2} 3 p^{4}$. In the exited state the available six orbitals i.e., one $s$, three $p$ and two $d$ are singly occupied by electrons. These orbitals hybridise to form six new $\mathrm{sp}^{3} \mathrm{~d}^{2}$ hybrid orbitals, which are projected towards the six corners of a regular octahedron in $\mathrm{SF}_{6}$. These six $\mathrm{sp}^{3} \mathrm{~d}^{2}$ hybrid orbitals overlap with singly occupied orbitals of fluorine atoms to form six S-F sigma bonds. Thus $\mathrm{SF}_{6}$ molecule has a regular octahedral geometry.
Q2 Explain formation of bonding and antibonding molecular orbital (L-II)
Ans Molecular orbitals may be described by the linear combination of atomic orbitals that can take place by addition and by subtraction of wave functions of individual atomic orbitals as shown below : $\psi \mathrm{MO}=\psi \mathrm{A}+\psi \mathrm{B}$ Therefore, the two molecular orbitals $\sigma$ and $\sigma^{*}$ are formed as: $\sigma=\psi \mathrm{A}+\psi \mathrm{B} \sigma^{*}$ $=\psi A-\psi B$. The molecular orbital $\sigma$ formed by the addition of atomic orbitals is called the bonding molecular orbital while the molecular orbital $\sigma^{*}$ formed by the subtraction of atomic orbital is called antibonding molecular orbital

Q3 Explain the formation of Lithium molecule on the basis of molecular orbital Also give its magnetic property.(L-I)
Ans. The electronic configuration of lithium is $1 s^{2}, 2 s^{1}$. There are six electrons in Li2. The electronic configuration of $\mathrm{Li}_{2}$ molecule, therefore, is $\mathrm{Li} 2:(\sigma 1 \mathrm{~s})^{2}\left(\sigma^{*} 1 \mathrm{~s}\right)^{2}(\sigma 2 \mathrm{~s})^{2}$ The above configuration is also written as $K K(\sigma 2 s)^{2}$ where $K K$ represents the closed $K$ shell structure $(\sigma 1 s)^{2}\left(\sigma^{*} 1 s\right)^{2}$.
Its bond order, therefore, is $1 / 2(4-2)=1$. It means that $\mathrm{Li}_{2}$ molecule is stable and since it has no unpaired electrons it should be diamagnetic.

Q4 Explain the diamagnetic behaviour of Hydrogen molecule on the basis of molecular orbital theory.(L-II)
Ans. It is formed by the combination of two hydrogen atoms. Each hydrogen atom has one electron in 1s orbital. Therefore, in all there are two electrons in hydrogen molecule which are present in o1s molecular orbital. So electronic configuration of hydrogen molecule is $\mathrm{H}_{2}$ : $(\sigma 1 \mathrm{~s})^{2}$. The bond order of $\mathrm{H}_{2}$ molecule can be calculated as given below:
Bond order $=\frac{1(N b-N a)}{2}=1$. This means that the two hydrogen atoms are bonded together by a single covalent bond

Q5 Explain the shape of $\mathrm{NH}_{3}$ molecule using hybridization. (L-I)
Bonding molecule orbital picture for ammonia, $\mathrm{NH}_{3}$


Lewis structure

Ans


## APPLICATION

## One mark Questions

Q1 What is the percentage of $s$ character in $\mathrm{sp}^{3}$ hybridizations? (L-I) Ans 25\%

Q2 What is the hybridization of carbon in carbon dioxide ? (L-I) Ans sp

Q3 Explain why ethyne molecule is linear?(L-II)
Ans It is because each carbon atom in ethyne is $s p$ hybridized
Q4 Name one compound each involving $\mathrm{sp}^{3}, \mathrm{sp}^{2}$, sp hybridization .(L-I)
Ans $\mathrm{sp}^{3}-\mathrm{CH}_{4}, \mathrm{sp}^{2}-\mathrm{C}_{2} \mathrm{H}_{4}, \mathrm{sp}-\mathrm{C}_{2} \mathrm{H}_{2}$

Q5 Which orbitals can overlap to form a sigma bond and which orbitals can do so to form a pi bond?(L-III)
Ans s-s, s-p, p-p can form sigma bond p-p can form pi bond

## Two marks Questions

Q1 Describe the change in the hybridization of the Al atom in the following reaction.(L-II)
$\mathrm{AlCl}_{3}+\mathrm{Cl}^{-} \rightarrow \mathrm{AlCl}_{4}^{-}$
Ans Hybridisation changes from $\mathrm{sp}^{2}$ to $\mathrm{sp}^{3}$

Q2 Is there any change in hybridization of B and N as a result of the reaction? (L-III)
$\mathrm{BF}_{3}+\mathrm{NH}_{3} \rightarrow \mathrm{BF}_{3} . \mathrm{NH}_{3}$
Ans Hybridisation of $B$ changes from $s p^{2}$ to $s p^{3}$ and that of nitrogen remains same as $s p^{3}$

Q3 Distinguish between atomic orbital and molecular orbital.(L-I)
Ans An atomic orbital is monocentric while a molecular orbital is polycentric.

Q4 Arrange the following in order of decreasing bond angles (L-II)
i) $\mathrm{CH}_{4}, \mathrm{NH}_{3}, \mathrm{H}_{2} \mathrm{O}, \mathrm{BF}_{3}, \mathrm{C}_{2} \mathrm{H}_{2}$
ii) $\mathrm{NH}_{3}, \mathrm{NH}_{2}{ }^{-}, \mathrm{NH}_{4}{ }^{+}$

Ans (i) $\mathrm{C}_{2} \mathrm{H}_{2}(180)>\mathrm{BF}_{3}(120)>\mathrm{CH}_{4}(109.28)>\mathrm{NH}_{3}(107)>\mathrm{H}_{2} \mathrm{O}(104.5)$
(ii) $\mathrm{NH}_{4}^{+}>\mathrm{NH}_{3}>\mathrm{NH}_{2}^{-}$,

Q5 Which d orbital is involved in $\mathrm{dsp}^{2}$ hybridization and why ?(L-III)
Ans $\mathrm{d}_{\mathrm{x}-\mathrm{y}}{ }^{2}$ because its four lobes lie along the x -axis and y axis. The two p orbitals can combine along these axis.

## Three marks Questions

Q1 Describe the shape of $\mathrm{PCl}_{5}$. Why axial bonds are longer than equatorial bonds in $\mathrm{PCl}_{5}$ ? (L-II) Ans $s p^{3} \mathrm{~d} \mathrm{P}-\mathrm{Cl}$ equatorial bond length is $2.04 \mathrm{~A}^{\circ}$ whereas $\mathrm{P}-\mathrm{Cl}$ axial is $2.19 \mathrm{~A}^{\circ}$ because repulsion exerted on axial bond pairs is more than equatorial bond


Trigonal bipyramidal structure of $\mathrm{PCl}_{5}$

Q2 Compare the relative stability of following species and indicate their magnetic properties .
$\mathrm{O}_{2}, \mathrm{O}_{2}^{+} \mathrm{O}_{2}^{-} \quad$ (L-I)
Ans. Stability increases as $\mathrm{O}_{2}{ }^{-}<\mathrm{O}_{2},<\mathrm{O}_{2}{ }^{+}$
Bond order $1 / 2,2,21 / 2$
Magnetic properties -Paramagnetic

Q3 What is the effect of the process $\mathrm{C}_{2} \rightarrow \mathrm{C}_{2}^{+}+\mathrm{e}^{-}$on bond order of $\mathrm{C}_{2}$ (L-II)
Ans. . Molecular Orbital Configuration of $\mathrm{C}_{2}$ is $\sigma_{1 s}{ }^{2} \sigma^{*}{ }_{1 s}{ }^{2} \sigma_{2 s}{ }^{2} \sigma^{*}{ }_{2 s}{ }^{2} \pi_{2 p y}{ }^{2} \pi_{2 p z}{ }^{2}$
$\mathrm{C}_{2}$ has bond order of 2 while that of $\mathrm{C}_{2}^{+}$is 1.5 so in process bond order decreases by 0.5

Q4 Draw and explain diagram showing hybridization in ethane(L-I)
Ans In the formation of ethene molecule, one of the $\mathrm{sp}^{2}$ hybrid orbitals of carbon atom overlaps axially with $\mathrm{sp}^{2}$ hybridised orbital of another carbon atom to form $\mathrm{C}-\mathrm{C}$ sigma bond. While the other two sp2 hybrid orbitals of each carbon atom are used for making $\mathrm{sp}^{2}-\mathrm{s}$ sigma bond with two hydrogen atoms. The unhybridised orbital (2px or $2 p y$ ) of one carbon atom overlaps sidewise with the similar orbital of the other carbon atom to form weak $\pi$ bond


Q5 Show the non-existence of helium molecule based on molecular orbital theory. (L-I)
Ans Helium molecule $\left(\mathrm{He}_{2}\right)$ : The electronic configuration of helium atom is 1s2. Each helium atom contains 2 electrons, therefore, in $\mathrm{He}_{2}$ molecule there would be 4 electrons. These electrons will be accommodated in $\sigma 1 \mathrm{~s}$ and $\sigma^{*} 1 \mathrm{~s}$ molecular orbitals leading to electronic configuration: $\mathrm{He} 2:(\sigma 1 \mathrm{~s})^{2}$ $\left(\sigma^{*} 1 \mathrm{~s}\right)^{2}$. Bond order of $\mathrm{He}^{2}$ is $1 / 2(2-2)=0$. $\mathrm{He}_{2}$ molecule is therefore unstable and does not exist.

