

## CHEMICAL BONDING AND MOLECULAR STRUCTURE

### Long Answer Questions:

1) What is meant by Hybridisation? Explain different types of Hybridisation involving S and P orbitals?

**Ans.** The process of mixing of suitable atomic orbitals of an atom resulting in the formation of new orbitals of similar shape and energy is called as hybridization of orbitals. The different types of hybridization, involving S & P orbitals are.

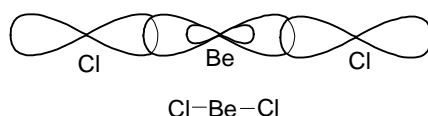
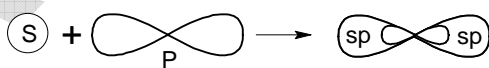
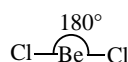
**SP hybridization:** One “s” orbital and one “p” orbital mix to form two “SP” hybrid orbitals. They have 50% “S” and 50% “p” character. Geometry of “SP” hybridized molecule is linear with bond angle  $180^\circ$ .

**Ex:**  $\text{BeCl}_2$

Electronic configuration of be in ground state is  $1s^2 2s^2 1s^2$

In excited state is  $1s^2 2s^1 2p^1$

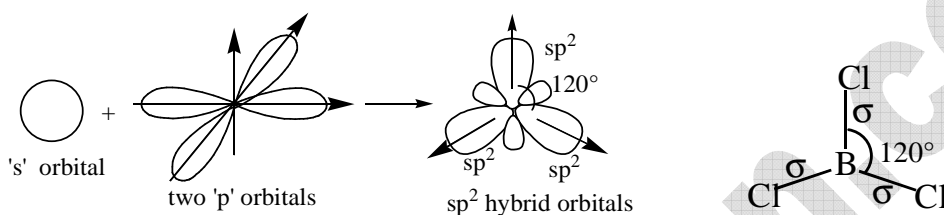
In the excited beryllium atom, ‘2s’ and ‘ $2p_x$ ’ orbitals intermix to give two equivalent ‘sp’ hybrid orbitals. The electronic configuration of Cl is  $1s^2 2s^2 2p^6 3s^2 3p_x^2 3p_y^2 3p_z^1$ . It has one half filled ‘p’ orbital. The half filled  $3p_z$  orbitals of two chlorine atoms overlap with ‘sp’ hybrid orbitals of beryllium atom in their axes to form two  $\sigma$  sp-p bonds.  $\text{BeCl}_2$  molecule has linear shape with bond angle  $180^\circ$ .



**$sp^2$  Hybridisation :** The intermixing of one ‘s’ orbital and two ‘p’ orbitals to form three  $sp^2$  hybrid orbitals. Each  $sp^2$  hybrid orbital has 33.33% ‘s’ character and 66.66% ‘p’ character. Geometry of “SP” hybridized molecule is trigonal planar with bond angle  $120^\circ$ .

**Ex;**  $\text{BCl}_3$

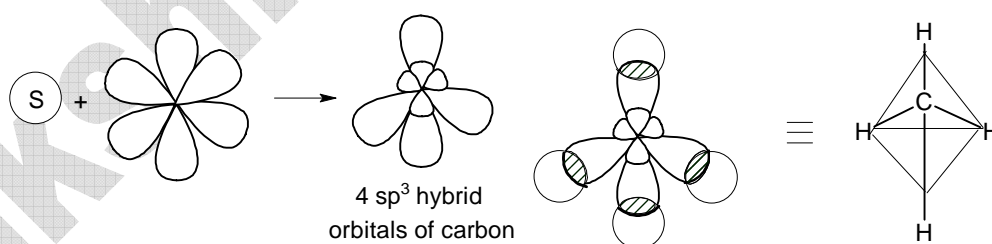
The central atom in  $\text{BCl}_3$  is boron. The electronic configuration of boron atom in its excited state is  $1s^2 2s^1 2p^2$  i.e.  $1s^2 2s^1 2p_x^1 2p_y^1$ . In the excited boron atom '2s' orbital and two '2p' orbitals intermix to give three equivalent  $sp^2$  hybrid orbitals. In the formation of  $\text{BCl}_3$  molecule, three  $sp^2$  hybrid orbitals of boron overlap with half filled  $3p_z$  orbitals of three chlorine atoms to give three  $\sigma sp^2$ -p bonds.  $\text{BCl}_3$  molecule has trigonal planar structure with bond angle  $120^\circ$ .



**$sp^3$  Hybridization:** The intermixing of one 's' orbital and three 'p' orbitals to give four equivalent  $sp^3$  hybrid orbitals is known as  $sp^3$  hybridisation. The four  $sp^3$  hybrid orbitals are directed towards the four corners of a regular tetrahedron. The angle between any two  $sp^3$  hybrid orbitals is  $109^\circ 28'$ .

**Ex: Methane Molecule**

The central atom in  $\text{CH}_4$  is carbon. The electronic configuration of carbon atom in its excited state is  $1s^2 2s^1 2p^3$  i.e.  $1s^2 2s^1 2p_x^1 2p_y^1 2p_z^1$

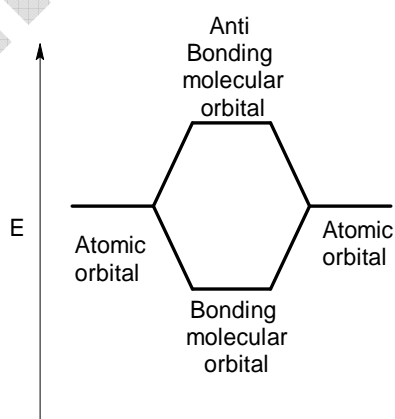


In the excited carbon atom, one '2s' orbital and three '2p' orbitals intermix to give four equivalent ' $sp^3$ ' hybrid orbitals. In the formation of methane molecule, four ' $sp^3$ ' hybrid orbitals of carbon overlap with '1s' orbital of four hydrogens to give four  $\sigma sp^3$ -s bonds. Methane molecule has tetrahedral shape with bond angle  $109.5^\circ$ .

## 2). Write the salient features of Molecular Orbital Theory?

**Ans.** Salient features of Molecular Orbital Theory developed by ‘**Hund** and **Mulliken**’ are

- 1) Electrons of atoms are present in atomic orbitals where as electrons of molecules are present in molecular orbitals.
- 2) The number of molecular orbitals formed will be equal to the number atomic orbitals combining.
- 3) The molecular orbitals whose energy is less than the atomic orbital are called as bonding molecular orbitals and the orbitals whose energy is more than the atomic orbitals are called as anti bonding molecular orbitals.
- 4) The molecular orbital, formed by the addition of atomic orbitals is called the bonding molecular orbital and by subtraction of atomic orbitals is called antibonding molecular orbital.
- 5) Stability of bonding molecular orbital is more than that of anti bonding molecular orbital.
- 6) The electron probability distribution in a molecule is given by molecular orbital.
- 7) The filling of electrons in molecular orbitals is similar to that of atomic orbitals i.e.: in accordance to Hund’s rule paulis exclusion principle and Aufbau’s principle.
- 8) Atomic orbitals are homocentric. i.e.: influenced only by one nucleus where as molecular orbitals is poly centric. i.e.: influenced by two nuclei
- 9) The combining atomic orbitals must have same or nearly same energy and same symmetry along axes

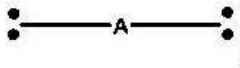
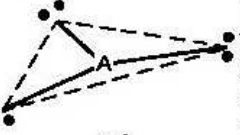
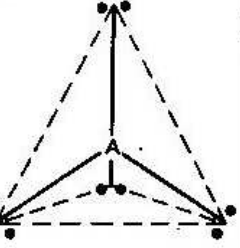
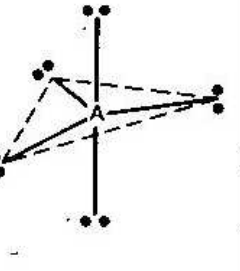
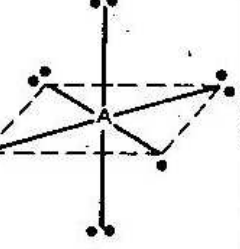


**3) What are the basic postulates of VSEPR theory? Discuss the shape of Methane and Ammonia molecules on the basis of VSEPR theory?**

**Ans.** Valence shell electron pair repulsion theory (VSEPR theory).

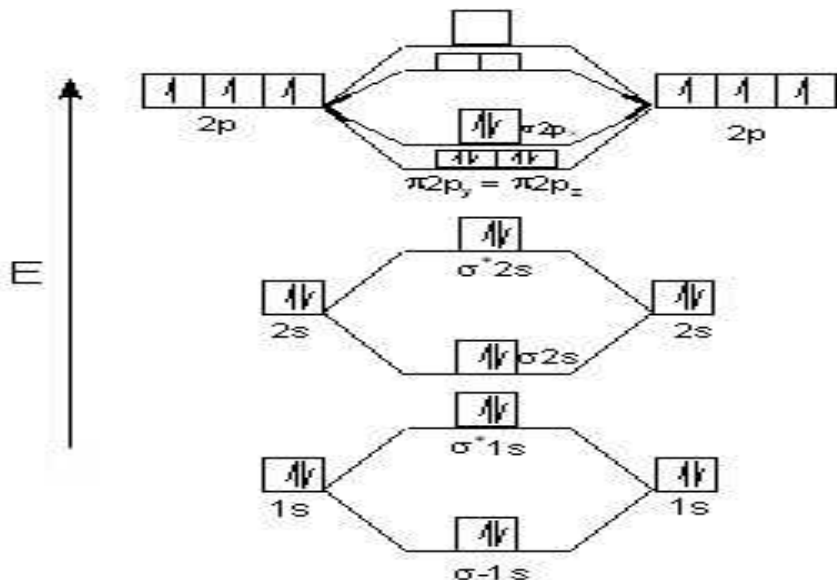
It was put forward by Sidgwick and Powell and later developed by Nyholm and Gillespie

- 1). It predicts the shapes of molecule based on the repulsive interactions between the electron pairs in valence shell of atoms.
- 2). The shape of the molecule depends on the number of bonded and non bonded electron pairs around central atom.
- 3). There is repulsion between electrons in valence shell as they are negatively charged.
- 4). To minimise repulsions the electrons tend to occupy positions with maximum separation between them.
- 5). The repulsive forces decrease in the order  $LP-LP > LP-BP > BP-BP$ .
- 6). The presence of lone pairs on the central atom causes slight distortion of the bond angles from the ideal shape. If the angle between a lone pair and the central atom and a bond pair is increased, it follows that the actual bond angle between the atoms must be decreased.

Valence Shell Electron Pairs	VSEPR Formula	Electron-Pair Orientation	Geometric Shapes	Bond Angles	Example
2	$AX_2$		linear	$180^\circ$	$HgCl_2$ , $BeCl_2$
3	$AX_3$		trigonal planar	$120^\circ$	$BF_3$ , $In(CH_3)_3$ , $C=$
	$AX_2E$		V-shaped		$SnCl_2$ , $PbBr_2$
4	$AX_4$		tetrahedral	$109.5^\circ$	$CH_4$ , $SnCl_4$ , $SiF_4$
	$AX_3E$		trigonal pyramidal		$NH_3$ , $PCl_3$ , $H_3O^+$
	$AX_2E_2$		V-shaped		$H_2O$ , $SCl_2$ , $OF_2$
5	$AX_5$		trigonal bipyramidal	$90^\circ$ , $120^\circ$	$PCl_5$ , $NbCl_5$
	$AX_4E$		irregular tetrahedral		$SF_4$ , $TeCl_4$
	$AX_3E_2$		T-shaped		$ClF_3$
	$AX_2E_3$		linear		$ICl_3$ , $XeF_2$
6	$AX_6$		octahedral	$90^\circ$	$SF_6$
	$AX_5E$		square pyramidal		$BrF_5$
	$AX_4E_2$		square planar		$ICl_4^-$ , $XeF_4$

4. Give the Molecular Orbital Energy diagram of a)  $N_2$  and  $O_2$ . Calculate the respective bond order. Write the magnetic nature of and molecules.

Ans.  $N_2$

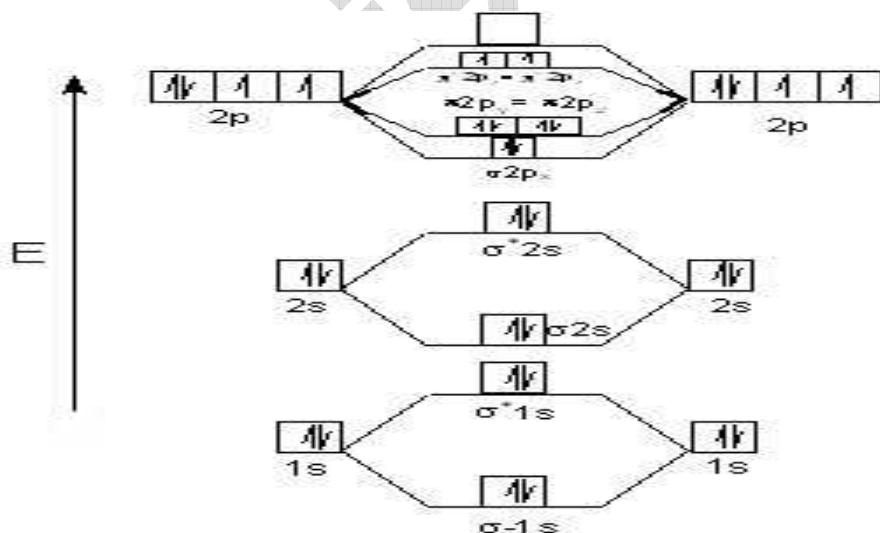


Electronic Configuration. Of  $N_2$   $(\sigma 1s)^2(\sigma^* 1s)^2(\sigma 2s)^2(\sigma^* 2s)^2(\pi 2p_x^2 = \pi 2p_y^2)(\sigma 2p_z)^2$

$$\text{Bond order} = \frac{N_b - N_a}{2} = \frac{10 - 4}{2} = 3$$

It is diamagnetic in nature as there are no unpaired electrons.

b)  $O_2$



EC of  $O_2 = (\sigma 1s)^2(\sigma^* 1s)^2(\sigma 2s)^2(\sigma^* 2s)^2(\sigma 2p_z)^2(\pi 2p_x^2 = \pi 2p_y^2)(\pi^* 2p_x^1 = \pi^* 2p_y^1)$

$$\text{Bond order in } O_2 = \frac{N_b - N_a}{2} = \frac{10 - 6}{2} = 2$$

O<sub>2</sub> molecule is paramagnetic in nature as there are 2 unpaired electrons.

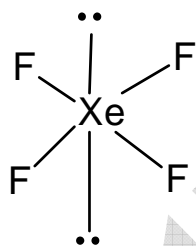
### Short Answer Questions

1. How do you predict the shapes of the following molecules making use of VSEPR theory?



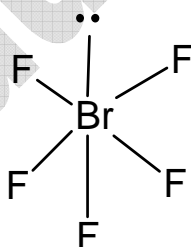
Ans. a) XeF<sub>4</sub>

It is AB<sub>4</sub>E<sub>2</sub> type of molecule. It has 4 B P and 2 LP. Hence the shape is square planar and arrangement is octahedral with two lone pairs.

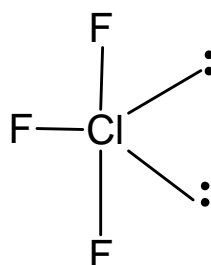


b) BrF<sub>5</sub>

It is AB<sub>5</sub>E type of molecule with 5 BP and 1 LP. Hence the shape is square pyramidal and arrangement is octahedral with one corner occupied by LP

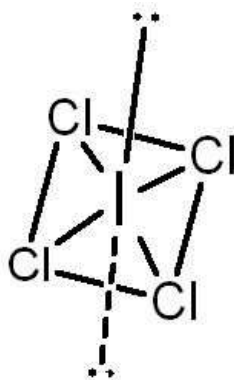


C) ClF<sub>3</sub>: It is AB<sub>3</sub>E<sub>2</sub> type of molecule with 3 bond pairs and 2 LP. Hence the shape is T-Shape and arrangement of electron pairs is Trigonal bipyramidal with two positions occupied by lone pairs.



d)  $\text{ICl}_4$ 

It is  $\text{AB}_4\text{E}_2$  type of molecule with 4 bond pairs and 2 lone pairs the shape is octahedral with 2 position occupied by lone pairs



## 2. Explain the formation of coordinate Covalent bond with one Example?

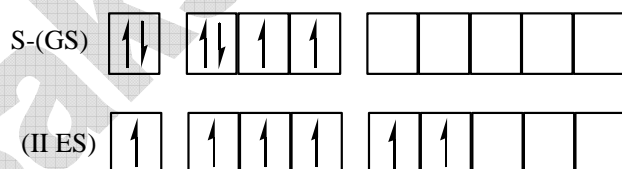
**Ans.** A covalent bond is formed by sharing a pair of electrons. A special type of covalent bond is formed in which the shared pair of electrons is contributed by one atom only. The atom which donates the shared pair of electrons is called as donor and that which accepts the electrons is called as acceptor. Such a bond results when a doubly filled orbital overlaps with an empty orbital of another atom. The bond between two atoms in which one donates a pair of electrons and the other accepts a pair of electrons is called as coordinate bond or dative bond.



Coordinate bond is shown by an arrow which is directed from donor to acceptor.

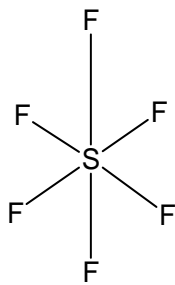
3. Explain the hybridization involved in  $\text{SF}_6$  molecule?

**Ans.**



One “s” and three “p” and two “d” orbitals of sulphur atom undergo  $sp^3d^2$  hybridisation. These  $6sp^3d^2$  hybrid orbitals overlap with 6 singly occupied p – orbitals of fluorine atoms to form  $6sp^3d^2 - P$  sigma bonds.





Shape is regular octahedron

#### 4. Define Dipole moment. Write its applications?

**Ans.** Dipole moment can be defined as the product of the magnitude of the charge and the distance between the charges. It is designed by  $\mu$ .

$$\mu = Q \times d$$

Where  $\mu$  dipole moment

Q is charge

D is distance (bond length)

It is expressed as de bye units (D) or coulomb meter (cm).

Dipole moment designated by a small arrow and it symbolizes the direction of shift of electron density in the molecule

#### Applications:

1) It is used to decide the polarity of the molecule. Molecules with zero dipole moment are non-polar and those with dipole moment are polar.

2) It is used to determine geometry of molecule.

**Ex:**  $CO_2$ ,  $BeF_2$  are linear as  $\mu=0$ .

3) It is also used to determine percentage of ionic character of a covalent bond.

### Very Short Answer

1. How many sigma and Pi bonds are present in a)  $C_2H_2$  and b)  $C_2H_4$

Ans. In  $C_2H_2$  number of sigma bonds are three and pi bond are two

In  $C_2H_4$  number of sigma bonds are five and pi bond is one

2. Which of the two ions  $Ca^{+2}$  (or)  $Zn^{+2}$  is more stable and why?

Ans.  $Ca^{+2}$  is more stable than  $Zn^{+2}$  because

$Ca^{+2}$  has octet configuration in valence shell where as  $Zn^{+2}$  has pseudo octet configuration in valence shell (18 electron configuration). Octet configuration is more stable than pseudo octet configuration.