



# **Chemical Bonding**

## **VSEPR Theory**

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## VSEPR Theory:

- VSEPR theory says that the shape of a given molecule (or) ion depends on the number and nature of electrons pairs surrounding the central atom(or) ion of the species.
- The main postulates of the theory is
- 1) spatial arrangement of electrons pairs round the central atom (or) ion of a given molecule (or)ion.
- 2)If the central atom is surrounded by two electrons i.e., if the sum of bonding electrons pairs (bps) and non-bonding electrons pairs also called lone pairs of electrons (lps) is two, their spatial arrangement is linear (diagonal) and the angle between them is  $180^{\circ}$
- 3)If the central atom is surrounded by 3 electron pairs( i.e.,bps+lps=3), their spatial arrangement is trigonal(or) triangular and if all the 3 electron pairs are bonding electron pairs the angle between each electron pairs is  $120^{\circ}$ .
- $\therefore$  Relation between the number of electrons pairs (i.e.,bps+lps) round the central atom, the spatial arrangement of the electrons pairs and bond angle (provided that all the electrons pairs are bonding electrons pairs i.e., there are no lone pairs are bonding electrons ) is shown as follows.

| No of electrons pairs (bps+lps)                               | 2             | 3                       | 4                | 5                           | 6            | 7                             |
|---|---------------|-------------------------|------------------|-----------------------------|--------------|-------------------------------|
| spatial arrangement of electrons pairs round the central atom | linear        | <u>Trigonal planner</u> | tetrahedral      | <u>Trigonal bipyramidal</u> | octahedral   | <u>pentagonal bipyramidal</u> |
| Bond angle  | $180^{\circ}$ | $120^{\circ}$           | $109^{\circ}28'$ | $120^{\circ}$               | $90^{\circ}$ | $90^{\circ}$                  |

## 4)Regular and irregular geometry:

- If the central atom is surrounded only by the bond pairs, then the molecule has a regular geometry. i.e., there is no distortion in the shape of the molecule.
- However if the central atom is surrounded by the bond pairs as well as lone pairs, the bond angle gets altered from the expected value.
- Therefore the presence of one (or) more lone pairs of electrons in the valence shell of the central atom gives irregular (or) distorted geometry of the molecule.

## Applications of VSEPR theory

### Shapes of Molecules

#### 1) shape of $\text{BeF}_2$ :

Atomic number of Be=4

Electronic configuration= $1s^2, 2s^2$

|                | 1s | 2s | 2p |
|----------------|----|----|----|
| Ground state:  | ↑↓ | ↑↓ |    |
| Excited state: | ↑↓ | ↑  | ↑  |

Be atom in ground state has electronic configuration  $1s^2, 2s^2$ . it has no unpaired electron and therefore should be chemically inert.

- However in the excited state, it has two unpaired electrons. Therefore Be atom can form two covalent bonds with fluorine atoms to give a molecule of beryllium fluoride F-Be-F.
- these hybrid orbitals must lie as far apart from each other as possible in order to minimize the force of repulsion between them and thus to have a stable structure.
- Hence, the two hybrid orbitals point in opposite directions. Therefore the molecule is linear and the F-Be-F bond angle is equal to  $180^\circ$





Other example:  $\text{BeH}_2$ ,  $\text{BeCl}_2$ ,  $\text{ZnCl}_2$  and  $\text{HgCl}_2$

## 2) Shape of $\text{BCl}_3$ :

Atomic number of B = 5

Electronic configuration =  $1s^2, 2s^2, p^1$

ground state:  $\uparrow\downarrow \quad \uparrow \quad \square \quad \square$

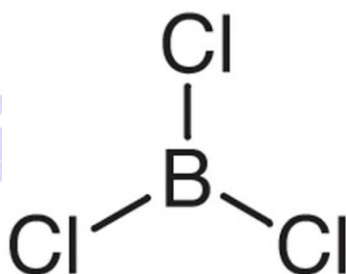
Excited state:  $\uparrow \quad \uparrow \quad \uparrow \quad \square$



$sp^2$  hybridization

In the excited state has 3 unpaired electrons. Now 3 covalent bonds can be resulting from  $sp^2$  hybridization of valence shell formed with 3 chlorine atoms giving a orbitals of the central boron atoms.

- According to VSEPR theory the three  $sp^2$  hybrid orbitals should be held at an angle of  $120^\circ$  to one another.
- This arrangement would lower the force of repulsion between electron pairs to the minimum.
- Since these three hybrid orbitals overlap with orbitals of three chlorine atoms, each Cl-B-Cl bond angle would be equal to  $120^\circ$  and therefore the molecule would be trigonal planner as shown in figure.



**Other examples:**  $\text{BH}_3$ ,  $\text{BF}_3$



## Shape of $\text{CCl}_4$

Atomic number of carbon=6

Electronic configuration= $1s^2, 2s^2, p^2$

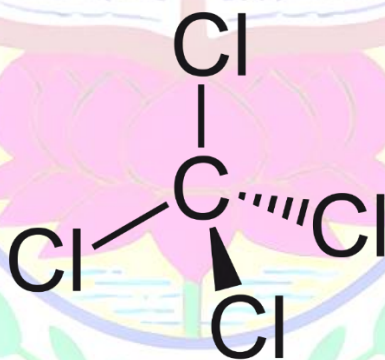
Ground state: 

Excited state: 

$sp^3$  hybridization

In the excited state c has four unpaired electrons therefore it can form four covalent bonds with Cl atoms to give a molecule of  $\text{CCl}_4$ .

- The one s and three p orbitals hybridize to give four  $sp^3$  hybrid orbitals of equal energy. If the orbitals are directed towards the four corners of a tetrahedron.
- Thus methane molecule has tetrahedral geometry. The C atom is at the centre of the tetrahedron and four chlorine atoms are at the four corners. The Cl-C-Cl bond angle is  $109^\circ 28'$

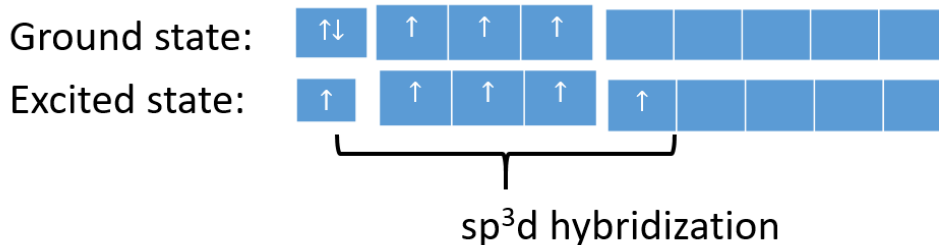


**Other example:**  $\text{CH}_4$ ,  $\text{SiF}_4$

## Shape of PF<sub>5</sub>:

Atomic number of P = 15

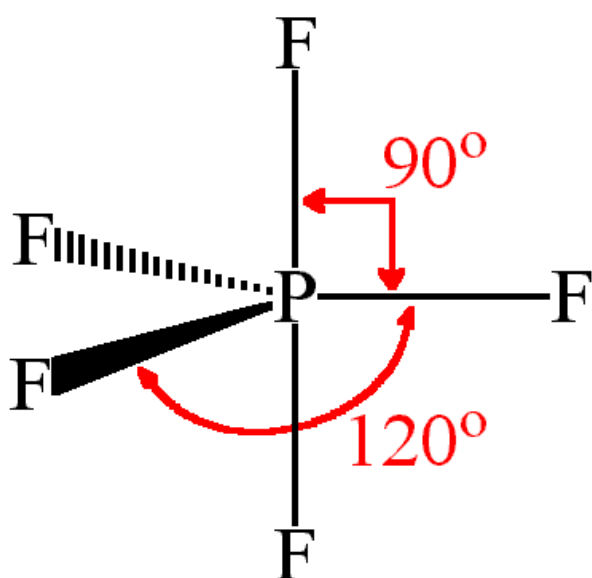
Electronic configuration:  $1s^2, 2s^2p^6, 3s^2p^3$



The formation of PF<sub>5</sub> is a case of sp<sup>3</sup>d hybridisation.

The centre p atom has the configuration  $3s^2p^3$  and has 3 unpaired electrons in the ground state .

In the excited state, one of electrons are promoted to 3d orbitals as shown in figure. The five sp<sup>3</sup>d hybrid orbitals (each singly filled with electron) thus obtained overlap with singly occupied orbitals of five F atoms and form five covalent bond. Since five hybrid orbitals are directed towards the 5 corners of a trigonal bipyramidal shape of PF<sub>5</sub> molecule and making an angle of 120° between them.



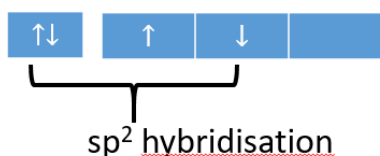
**Others examples:** PCl<sub>5</sub>, SbCl<sub>5</sub>

## Shape of SnCl<sub>2</sub>:

Atomic number of Sn = 50

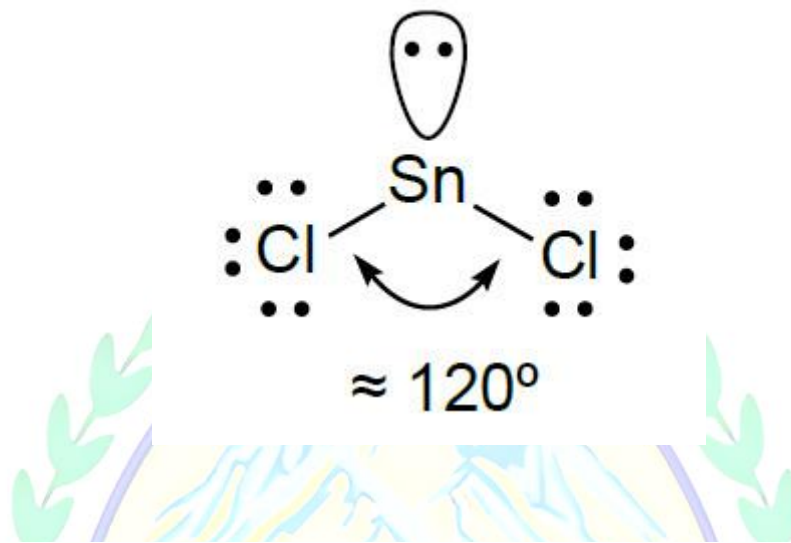
Electronic configuration =  $1s^2, 2s^2p^6, 3s^2p^6d^{10}, 4s^2p^6d^{10}, 5s^2p^2$

Ground state:



The outer electronic configuration of the central Sn atom is  $5s^2, 5p_x^1, p_y^1$ . There are two unpaired electrons in 5p orbitals of tin and these are sufficient to form two bonds with Cl atoms and therefore there is no need of promotion of electrons.

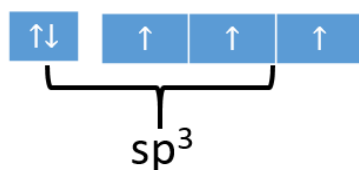
- The bond formation can take place by the overlapping of the two mutually perpendicular half-filled  $p_x$  and  $p_y$  orbitals of tin atom with the half-filled p orbitals of the two Cl atoms.
- Thus the molecule should be angular with Cl-Sn-Cl bond angle equal to  $90^\circ$ .
- Hence, it has been postulated that one-s and two p orbitals of tin hybridize to give three  $sp^2$  hybrid orbitals of equivalent energy.
- These  $sp^2$  hybrid orbitals are arranged around the central atom in a trigonal planar geometry one of these hybrid orbitals contains a lone pair of electrons.
- Thus the central atom Sn in SnCl<sub>2</sub> is surrounded by three orbitals, each containing a pair of electrons.
- Two of these orbitals contain bond pairs while the third contains a lone pair of electrons. The geometry of the molecule should have been V-shaped with bond angle of  $120^\circ$ .



### Shape of NH<sub>3</sub>:

Atomic number of N=7

Electronic configuration=1s<sup>2</sup>,2s<sup>2</sup>2p<sup>3</sup>



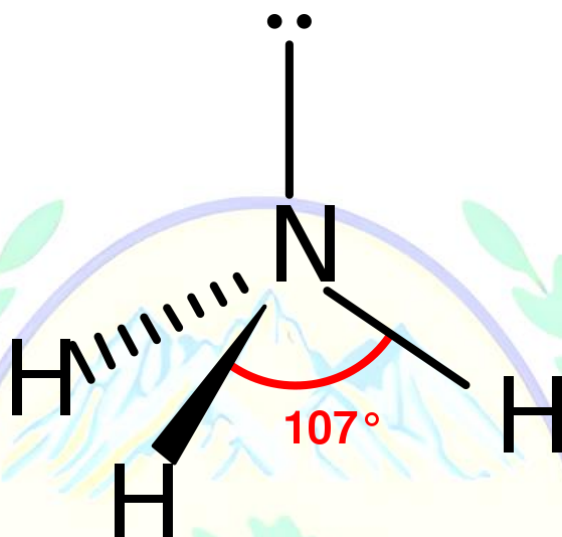
Out of its 5 valance electrons of N atom three are used up in forming three sigma bonds with three hydrogen atoms while the remaining two electrons(i.e., 1 electron pair) remain as non-bonding electrons on N-atom.

Sigma bond pairs=3 and lone pairs=1 and sigma bond pairs+ lone pairs=4.

- Now since the sum of sigma bond pairs and lone pairs is 4, N atom in NH<sub>3</sub> molecule is supposed to be sp<sup>3</sup> hybridized as shown in figure.
- The hybrid orbital containing the lone pair does not participate in the overlapping (or)N-H sigma bond formation process while the singly filled sp<sup>3</sup> hybrid orbitals make a linear overlap with the



singly filled 1s orbital on each of the three H- atoms ( $H-1s^1$ ) and from 3 sigma bonds as shown in figure



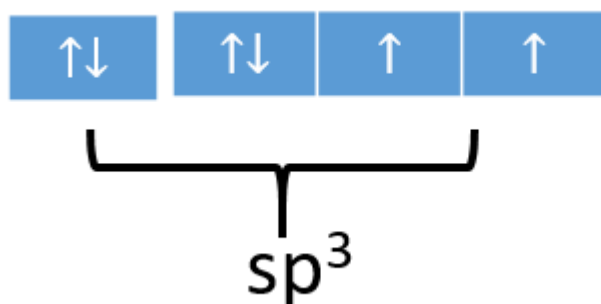
Due to the presence of one lone pair of electrons , the shape of  $NH_3$  molecule gets distorted and becomes trigonal pyramidal and each of 3 H-N-H bond angle decrease from the expected tetrahedral shape ( $109.5^\circ$  to  $107^\circ$ ). This distortion in shape and reduction in the bond angle can be explained on the basis of VSEPR theory.

### Shape of $H_2O$ :

Atomic number of oxygen=8

Electronic configuration= $1s^2, 2s^2p^4$

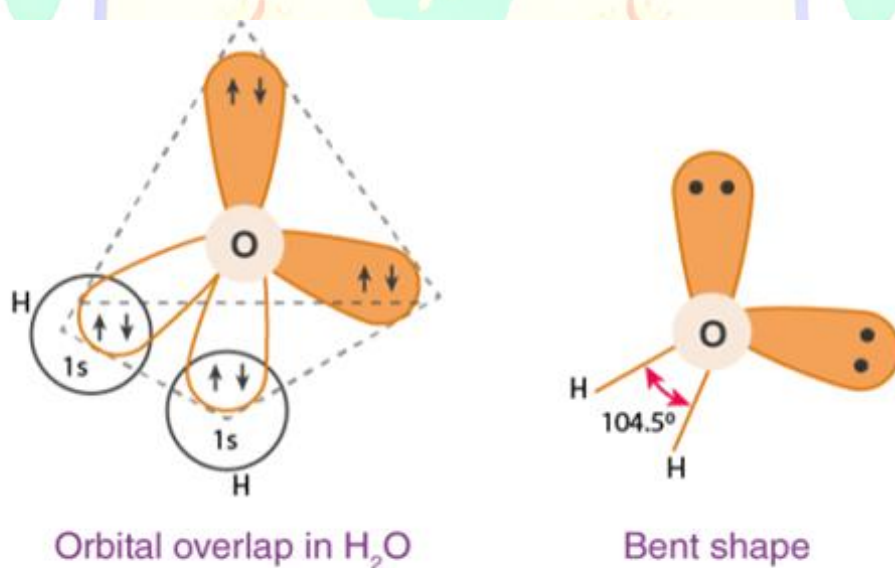
Ground state:



- In  $H_2O$  molecule, the central atom is O. its outer electronic configuration is  $2s^22p_x^2p_y^1p_z^1$  as represented in figure. Thus there are two unpaired electrons which can form two bonds with H-

atoms while the remaining 4 electrons (i.e., 2 electron pairs) remain as lone pair of electrons on O atom.

- Thus sigma bond pairs =2 and lone pairs =2 and hence sigma bond pairs + lone pairs = 4.
- Since the sum of sigma bond pairs and lone pairs is 4, O atom in H<sub>2</sub>O molecule is supposed to be sp<sup>3</sup> hybridization as shown in figure.
- According to VSEPR theory, these hybrid orbitals are arranged tetrahedrally around the O- atom.
- Due to the presence of two lone pairs of electrons in two hybrid orbitals, the shape of H<sub>2</sub>O molecules get distorted and becomes V-shape (angular(or) bent shape) and H-O-H bond angle decrease from the expected tetrahedral bond angle(=109.5<sup>0</sup>) to 104.5<sup>0</sup>



KNOWLEDGE