SHAPES OF SIMPLE MOLECULES

(Valance shell Electron Pair Repulsion Theory)

VSEPR Theory

For maximum stability of a molecule the orbitals occupied by electrons in the valency shell of the central atom, should be so arranged in space that they lie as far away from one another as possible. The theory may also be given in the form of pastulates :

i. In the formation of simple covalent molecule, there is one central atom which forms covalent bonds with other atoms.

ii. In the formation of covalent bonds, orbitals get occupied by electron pairs. When a central atom forms more than one covalent bond there will be more than one such orbitals surrounding the central atom.

iii. Since electrons experience electrostatic repulsion from one another the orbitals containing electrons also experience similar electrostatic repulsions. The orbitals, therefore, tend to keep apart from one another as far as possible.

Explanation :

i. In the formation of a molecule of water the central atoms is oxygen which forms two covalent bonds with two hydrogen atoms. Similarly in ammonia nitrogen is the central atom and in methane carbon is the central atom. Similarly every molecule will have one central atom. It will be surrounded by one or more covalent bonds.

ii. Each bond surrounding the central atom will have a pair of electrons

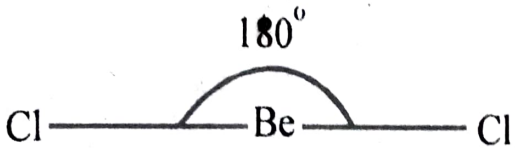
iii. The electron pairs in the covalent bons repel each other. Because of this repulsion, the bonds tend to keep away from one another, so that they experience minimum repulsion. This provides them definite shape.

This theory applies not only to the orbitals contaning shared pairs of electrons but also to the orbitals containing lone pairs of electrons This arrangement of orbitals in space minimises the force of repulsion between them. The molecule, therefore, has minimum energy and maximum stability.

SHAPES OF SIMPLE INORGANIC MOLECULES

1. Linear :

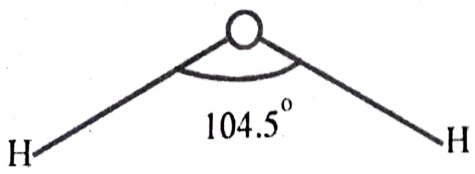
If there are only two orbitals present around the central atom in a molecule, the only way to keep them far apart is to arrange them **linearly** i.e., with an angle 180°. Example : Beryllium chloride Cl – Be – Cl. The shape of the molecule is shown in figure. $HgCl_2$ and BeF_2 are other examples.



2. Bent structure :

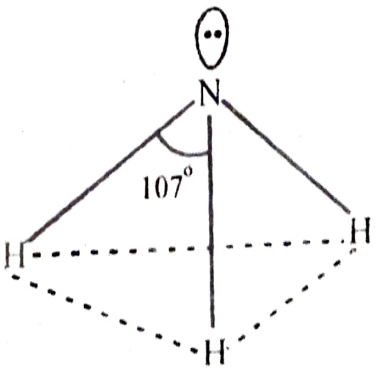
In water molecule, the oxygen atom has two bonding electron pairs and two lone pairs. The electrostatic repulsions between them lead to a tetrahedral arrangement. The bonds of the O atom will be directed to the two corners of a tetrahedran and the lone pairs towards the other two.

Since the non bonding electrons, repel more strongly than the bonding electrons, the two bonds will be forced closer. Thus the normal tetrahedral angle (109°28') is reduced to 104.5°. The water molecule, assumes a V - shaped **bent structure** as shown in figure.



3. Pyramidal :

In **ammonia** molecule, the N atom has three bonding electron pairs and one lone pair. Because of electrostatic repulsions, it is expected that the three covalent bonds will be directred to the three corners of a tetrahedron while the lone pair will be directed towards the fourth corner.

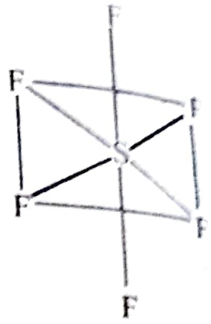


According to VSEPR theory, a lone pair exerts a greater repulsion on the bonding pairs. As a result, the three bonds of NH_3 molecule are forced slightly closer together leading to a **pyramidal structure** with the lone pair at the top as shown in figure.

Another example : ClF_3

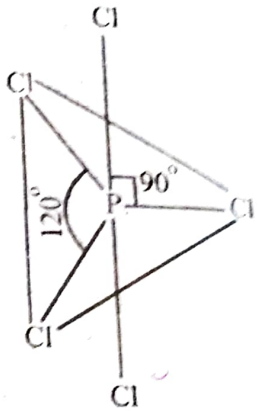
4. Octahedral :

If there are six orbitals around the central atoms of the molecule , the molecule has the shape of a **regular octahedron**. The bond angle is 90°. Sulphur hexafluoride is an example for this type. The structure is shown figure.



5. Trigonal bipyramidal :

If there are give orbitals around the central atom in a molecule the only way to keep them far apart is to arrange them in **trigonal bipyramidal** structure. Phosphorous pentachloride PCl_5 is an example for this type and the structure is shown in figure.



6. Pentagonal bipyramid :

If there are seven orbitals around the central atom of the molecule, the molecule has the shape of **pentagonal bipyramid**. Iodine hepta fluride, IF_7 is an example for this type. This is shown in figure. XeF_6 also has similar structure. But one position is occupied by a lone pair of electrons.