Chemistry Study Materials for Class 11 (NCERT Based Notes of Chapter- 04)

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CHEMICAL BONDING AND MOLECULAR STRUCTURE

The shapes of molecules

Covalent bonds are directional in nature. i.e. they are directed to some specified positions in space. So covalent compounds have definite shapes.

The Valence Shell Electron Pair Repulsion [VSEPR] Theory

This theory was proposed by Sidgwick and Powell and later modified by **Nyholm and Gillespie.** The important postulates of this theory are:

1) The shape of the molecule depends on the number of valence shell electron pairs (VSEPRs) around the central atom.

2) The valence shell electron pairs repel each other.

3) In order to reduce the repulsion, the electron pairs stay at maximum distance.

4) Presence of lone pairs of electron causes distortion in the expected geometry of the molecule.

The repulsion between two lone pairs of electrons is different from those between two bond pairs or between a lone pair and bond pair. The repulsion decreases in the order lone pair –

lone pair > lone pair - bond pair > bond pair - bond pair.

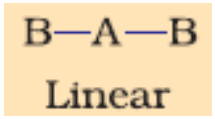
5) As the angle between the electron pairs increases, the repulsion decreases.

Prediction of geometry of molecules using VSEPR theory

I) Molecules containing only bond pairs of electrons

1) **AB_2 type** (where A is the central atom and B is the no. of bond pairs)

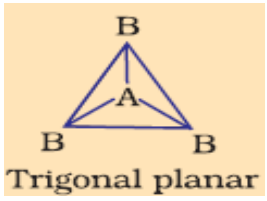
Here there are 2 VSEPs. In order to reduce the repulsion, these electron pairs are arranged at an angle of 180^0. Thus the shape of the molecule is linear with bond angle 180^0.



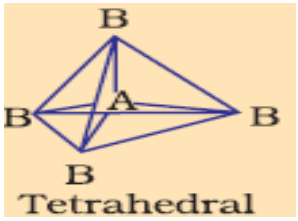
e.g. $BeCl_2$, $HgCl_2$ etc.

2) **AB_3 type**: Here there are 3 VSEPs. In order to reduce the repulsion, these electron pairs are arranged at an angle of 120^0. Thus the shape of the molecule is planar triangular (trigonal planar) with bond angle 120^0.

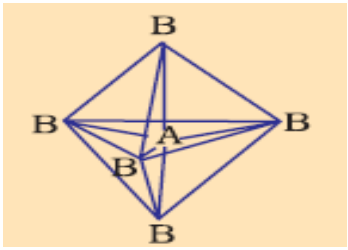
e.g. BF_3, BCl_3 etc.



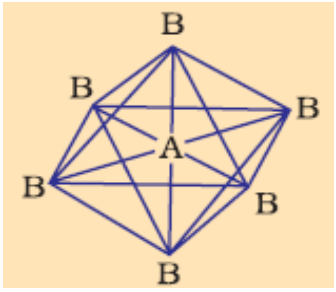
3) **AB_4 type**: Here there are 4 VSEPs. These are arranged at the four corners of a tetrahedron and hence the shape of the molecule is tetrahedral with bond angle 109^028^l. e.g.: CH_4, NH_4+ etc.



4) **AB_5 type**: Here there are 5 VSEPs. To reduce the repulsion, they are arranged at the five corners of a trigonal bipyramid with bond angles 120^0 and 90^0.
E.g. PCl_5



5) **AB_6 type:** Here there are 6 VSEPs. To reduce the repulsion, they are arranged at the six corners of an octahedron with bond angles 90^0. E.g.: SF_6



II) Molecules containing both bond pairs and lone pairs

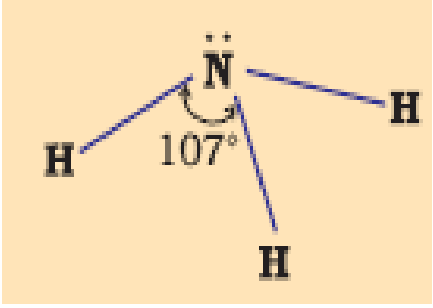
The presence of lone pairs of electron causes distortion in the shape of the molecules.

Type of molecule	Total no. of VSEPs	No. of b.ps	No. of l.ps	Shape	e.g.
AB_2E	3	2	1	Bent	SO_2, O_3
AB_3E	4	3	1	Trigonal Pyramid	NH_3
AB_2E_2	4	2	2	Bent	H_2O
AB_4E	5	4	1	See-saw	SF_4
AB_3E_2	5	3	2	T-Shape	ClF_3
AB_5E	6	5	1	Square Pyramid	BrF_5
AB_4E_2	6	4	2	Square Planar	XeF_4

Explanation of shapes of ammonia and water molecules by VSEPR theory

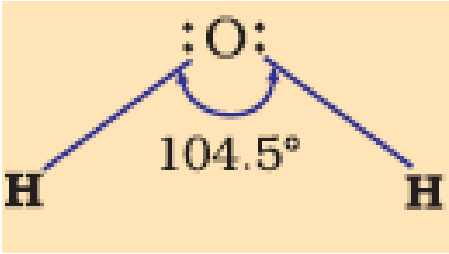
1. NH_3

In ammonia, the central atom N has 5 valence electrons ($_7N$ – 2,5). Among these electrons, three are used for the formation of bonds with hydrogen atoms and the remaining 2 electrons stay as lone pairs. So there are 4 VSEPs. Hence the expected shape of the molecule is tetrahedral. But due to the presence of lone pairs, the shape is distorted to trigonal bipyramidal and the bond angle changes from $109^0 28^l$ to 107^0.



2. H_2O

In water, the central atom O has 6 valence electrons ($_8O$ – 2,6). Two of them are used for the formation of bonds with hydrogen atoms and the remaining 4 electrons stay as lone pairs. So there are 4 VSEPs. Hence the expected shape of the molecule is tetrahedral. But due to the presence of 2 lone pairs, the shape is distorted bent or angular or inverted v shape and the bond angle changes from $109^0 28^l$ to 104.5^0.



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