VSEPR (Valence shell electron pair repulsion) theory.

The basic concept of the theory was suggested by Sidgwick and Powell (1940). It provides useful idea for predicting shapes and geometries of molecules. The concept tells that, the arrangement of bonds around the central atom depends upon the repulsion's operating between electron pairs(bonded or non bonded) around the central atom. Gillespie and Nyholm developed this concept as VSEPR theory.

The main postulates of VSEPR theory are

(i) For polyatomic molecules containing 3 or more atoms, one of the atoms is called the central atom to which other atoms are linked.

(ii) The geometry of a molecule depends upon the total number of valence shell electron pairs (bonded or not bonded) present around the central atom and their repulsion due to relative sizes and shapes.

(iii) If the central atom is surrounded by bond pairs only. It gives the symmetrical shape to the molecule.

(iv) If the central atom is surrounded by lone pairs (lp) as well as bond pairs (bp) of e^- then the molecule has a distorted geometry.

(v) The relative order of repulsion between electron pairs is as follows : Lone pair-lone pair>lone pair-bond pair>bond pair-bond pair

A lone pair is concentrated around the central atom while a bond pair is pulled out between two bonded atoms. As such repulsion becomes greater when a lone pair is involved.

Steps to be followed to find the shape of molecules :

(i) Identify the central atom and count the number of valence electrons.

(ii) Add to this, number of other atoms.

(iii) If it is an ion, add negative charges and subtract positive charges. Call the total N.

(iv) Divide N by 2 and compare the result with the following table and obtain the shape.

Total N/2	Shape of molecule or ion	Example
2	Linear	$HgCl_2$ / $BeCl_2$
3	Triangular planar	BF_3
3	Angular	$SnCl_2, NO_2$
4	Tetrahedral	CH_4, BF_4^-

4	Trigonal Pyramidal	NH_3, PCl_3
4	Angular	H_2O
5	Trigonal bipyramidal	PCl_5, PF_5
5	Irregular tetrahedral	SF_4, IF_4^+
5	T-shaped	ClF_3, BrF_3
5	Linear	XeF_2, I_3^-
6	Octahedral	SF_6, PF_6
6	Square Pyramidal	IF_5
6	Square planar	XeF_4, ICl_4

Geometry of Molecules/Ions having bond pair as well as lone pair of electrons

Type of mole-cule	No. of bond pairs of electron	No. of lone pairs of electrons	Hybridi-zation	Bond angle	Expected geometry	Actual geometry	Examples
AX_3	2	1	sp^2	< 120o	Trigonal planar	V-shape, Bent, Angular	SO_2, $SnCl_2$, NO_2^-
AX_4	2	2	sp^3	< 109o 28′	Tetrahedral	V-shape, Angular	H_2O, H_2S, SCl_2, OF_2, NH_2^-, ClO_2^-
AX_4	3	1	sp^3	< 109o 28′	Tetrahedral	Pyramidal	NH_3, NF_3 , PCl_3, PH_3, AsH_3, ClO_3^- , H_3O^+
AX_5	4	1	sp^3d	< 109o 28′	Trigonal bipyramidal	Irregular tetrahedron	SF_4, SCl_4, $TeCl_4$
AX_5	3	2	sp^3d	90o	Trigonal bipyramidal	T-shaped	ICl_3, IF_3, ClF_3
AX_5	2	3	sp^3d	180o	Trigonal bipyramidal	Linear	XeF_2, I_3^-, ICl_2^-
AX_6	5	1	sp^3d^2	< 90o	Octahedral	Square	ICl_5, BrF_5, IF_5

						pyramidal	
AX_6	4	2	sp^3d^2	–	Octahedral	Square planar	XeF4, ICl4–
AX7	6	1	sp^3d^3	–	Pentagonal pyramidal	Distorted octahedral	XeF6