

V.S.E.P.R Theory

Valence shell Electron Pair Repulsion Theory.

The idea of a Correlation between molecular geometry and number of valence (shell) electron pairs (Both B.P & H.P) was originally proposed in 1939 by R. Tsuchimoto (Japan). In 1940, it was intro. presented by Sidgwick and Powell in university of Oxford.

In 1957 Ronald Gillespie and Ronald S. Nyholm of university - College London refined this concept into a more detailed theory.

Valence shell electron pair repulsion theory is a model used to predict the Geometry of individual molecule in three dimensional space on the basis of numbers of electron pairs surrounding Central atom.

The Premise of V.S.E.P.R Theory is that - the valence electron pair surrounding an atom, to repel each other and, will, therefore adopt an arrangement that - minimise this repulsion, so, it decreases the energy of a molecule and increases the stability of molecules.

or in other words it explains the shape of simple molecules and ions on the basis of repulsions among the electron pairs present in the valence shell of their Central atoms.

This theory may be pointed as follows,

- (1) Valence electrons of the Central atom of molecules or ions form pairs with anti-parallel spins. Each electron pair occupies a reasonably well defined region in the space and other electron pairs are effectively excluded from this space.

(2) The electrons already present in valence (outermost) shell and the additional electrons acquired by the central atom as a result of bonding with others are called valence electrons or valence shell electrons.

(3) These electron pairs stay as far apart from one another in space as possible to minimise the mutual repulsions to form stable geometrical shape or arrangement.

4. The most stable geometrical arrangement of, two, three, four, five & six (2, 3, 4, 5, & 6) electron pairs is linear, trigonal planar, tetrahedral, trigonal bi-pyramidal and Octahedral respectively.

5. Some or all electron pairs may be involved in bondings called Bond Pairs (B.P.) while others are called lone pairs (L.P.) or non-bondings.

6. If the central atom in molecule is surrounded by only bond pairs then the molecule has regular or symmetrical geometry but in case of BPs and LPs, the molecule does not have regular geometrical shape e.g. in CH_4 , the four sp^3 hybridised orbitals have bond pairs resulting in a symmetrical tetrahedral shape.

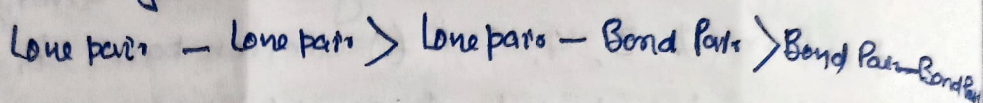
As in case of NH_3 , H_2O & HF have one, two and three lone pairs on the central atoms, hence they have Pyramidal, Angular and Linear shape respectively, but not the tetrahedral shape, though they have the same sp^3 hybridisation and tetrahedral structure.

7. A lone pair occupies more space on the surface of the central atom than a bond pair because a bond pair is attached by two nuclei and the lone pair is attached by only one nucleus.

Hence bond order of decreasing repulsion as



∴ Electrostatic repulsion between L.P. & B.P. is in the following order.



Now the increasing repulsion decreases the bond angle.

Molecule: -	CH ₄	NH ₃	H ₂ O
Hybridisation: -	sp ³	sp ³	sp ³
Structure: -	Tetrahedral	Tetrahedral	Tetrahedral
No. of B.Ps	4	3	2
No. of L.Ps	0	1	2
Repulsion between electron pairs	Increases		

Bond angle.

109.5°

107.3°

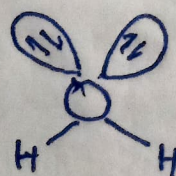
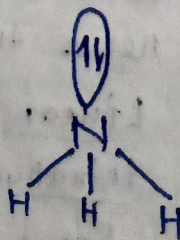
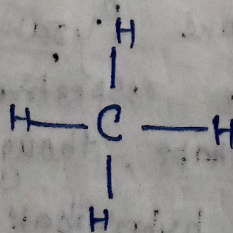
104.5°

→

Decreases

→

Decreases



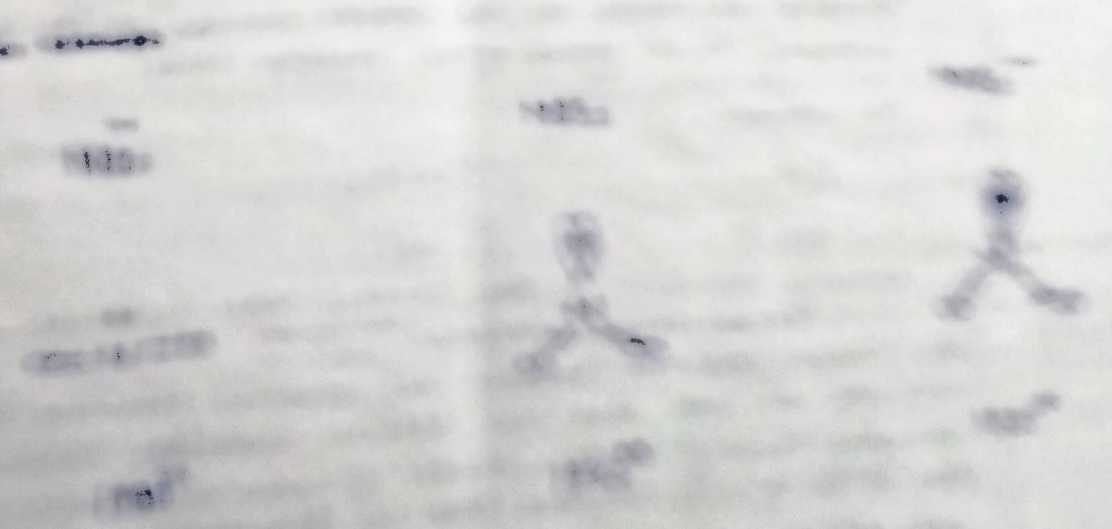
10. The first part of the paper is devoted to the study of the properties of the function $f(x)$ defined by the equation

$$f(x) = \begin{cases} x^2 & \text{if } x \in [0, 1] \\ 2x - 1 & \text{if } x \in (1, 2] \end{cases}$$

It is easy to see that the function $f(x)$ is continuous on the interval $[0, 2]$. In fact, for $x \in [0, 1]$, the function is a polynomial, and for $x \in (1, 2]$, the function is a linear function. At the point $x = 1$, we have $f(1) = 1$ and $\lim_{x \rightarrow 1} f(x) = 1$, so the function is continuous at $x = 1$. Therefore, the function $f(x)$ is continuous on the entire interval $[0, 2]$.

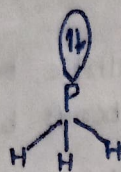
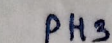
x	$f(x)$
0	0
1	1
2	3

4. Let us now consider the function $g(x)$ defined by the equation

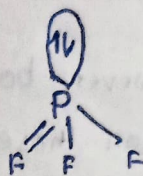


10. A lone pair and single bond repulsion is larger than a lone pair and double bond repulsion.

For example:



99.3°



104°

11. The Size of Bonding Pair on A decreases with increasing electronegativity of B.

In other words the bond angle in compounds having formula AB_n increases as the electronegativity of B decreases.

For example:-



Bond angle:- 100°



101.5°



102°

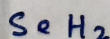
i.e. $\rightarrow$ electronegativity of X = Cl, Br, I decreases $\rightarrow$ decreases $\rightarrow$
Bond angle increases:- increases $\rightarrow$

12. The bond angle in compounds having same empirical formula decreases as the atomic numbers of the Central atom increases in a group of the periodic table.

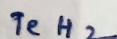
For example:-



92.5°



91°



89.5°

Atomic number of the central atom increases $\rightarrow$
Bond angle decreases $\rightarrow$

Defect:- This theory does not predict the detailed structure of unsymmetrical molecules or ions and the species involving central atoms formally having valence shells of more than twelve electrons, thus it is of only limited help in interpreting a complicated state of affairs. It also does not explain the angular shape of some gaseous alkali earth halides and alkali metal oxides i.e. Li2O as they do not have any electron pair on the metal atom. If LP-LP repulsions are strongest, H2H2 should have anti-not gauche configuration.