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VSEPR THEORY(VALENCE SHELL ELECTRON PAIR. REPULSION THEORY)

What is VSEPR Theory?

VSEPR theory was developed in 1947 by Gillespie andNyholm .This theory predicts molecular shape and bond angles more accurately.It states that "*the lone pair and shared pair arrange themselves around the central atom in space as far apart as possible to minimize the electrostatic force of repulsion.*"

The Valence Shell Electron Pair Repulsion Theory abbreviated as VSEPR theory is based on the premise that there is a repulsion between the pairs of valence electrons in all atoms, and the atoms will always tend to arrange themselves in a manner in which this electron pair repulsion is minimalized. This arrangement of the atom determines the geometry of the resulting molecule.

Postulates of VSEPR Theory:

The postulates of the VSEPR theory are listed below:--

1. Total number of electron pairs around the central atom = ½ (number of valence electrons of central atom + number of atoms linked to central atom by single bonds)

- For negative ions, add the number of electrons equal to the units of negative charge on the ions to the valence electrons of the central atom.
- For positive ions, subtract the number of electrons equal to the units of positive charge on the ion from the valence electrons of the central atom.

2. The number of Bond pair = Total number of atoms linked to central atom by single bonds.

3. Number of lone pairs = Total number of electron – No of shared pair

The electron pairs around the central atom repel each another and move so far apart from each another that there are no greater repulsions between them. This results in the molecule having minimum energy and maximum stability.

- The shape of a molecule with only two atoms is always linear.
- For molecules with three or more atoms, one of the atoms is called the central atom and other atoms are attached to the central atom.
- If the central atom is linked to similar atoms and is surrounded by bond pairs of electrons only, the repulsions between them are similar as a result the shape of the molecule is symmetrical and the molecule is said to have regular geometry.

- If the central atom is linked to different atoms or is surrounded by bond pair as well as a lone pair of electrons, the repulsion between them is similar. As a result, the shape of the molecule has an irregular or distorted geometry.
- The exact shape of the molecule depends upon the total number of electron pairs present around the central atom.

The following terms are commonly used in discussing the shapes of molecules.

- **Bond Angle:** This is the angle between a bonded atom, the central atom, and another bonded atom.
- **Lone Pair:** This refers to a pair of valence electrons that are not shared with another atom.
- **Molecular Geometry:** This is the 3-D arrangement of bonded atoms in a polyatomic ion or molecule.
- **Electron Pair Geometry:** This is the 3-D arrangement of electron pairs around the central atom of a polyatomic ion or molecule.

Using the VSEPR Chart to Determine Shape and Bond Angle

To use a VSEPR table, first determine the coordination number or number of electron pairs.

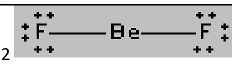
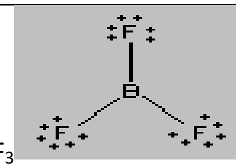
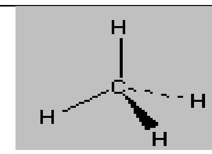
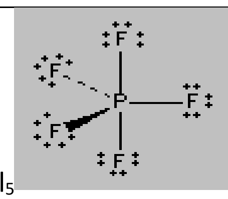
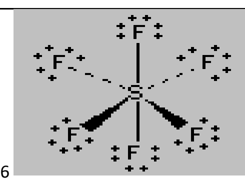
1. Count the valence electrons of the central atom.
2. Add an electron for each bonding atom.
3. Subtract an electron if the central atom has a positive charge; and add an electron for a central atom with negative charge.
4. Halve your count to get the total electron pairs.

Finally, look up your molecule on the chart by coordination number and number of atoms.

Alternatively, you can count the lone electron pairs, which are also indicated on the chart.

Example: PCl_5

Once you know PCl_5 has five electron pairs, you can identify it on a VSEPR chart as a molecule with a trigonalbipyramidal molecular geometry. Its bond angles are 90° and 120°, where the equatorial-equatorial bonds are 120° apart from one another, and all other angles are 90°.

VSEPR Number	Shape of the Molecule	VSEPR Number	Shape& Structure
2	Linear	2	BeF_2 
3	Trigonal Planar	3	BF_3 
4	Tetrahedral	4	CH4 
5	TrigonalBipyramidal	5	PCl_5 
6	Octahedral	6	SF_6 

Limitations of VSEPR Theory:

Some significant limitations of the VSEPR theory include:

- This theory fails to explain isoelectronic species (i.e. elements having the same number of electrons). The species may vary in shapes despite having the same number of electrons.
- The VSEPR theory does not shed any light on the compounds of transition metals. The structure of several such compounds cannot be correctly described by this theory. This is because the VSEPR theory does not take into account the associated sizes of the substituent groups and the lone pairs that are inactive.
- Another limitation of VSEPR theory is that it predicts that halides of group 2 elements will have a linear structure, whereas their actual structure is a bent one.

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