13.13: Molecular Structure: The VSEPR Model

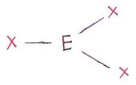
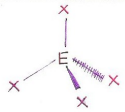
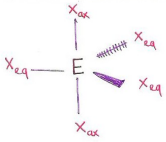
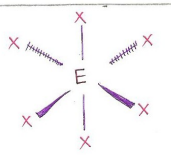
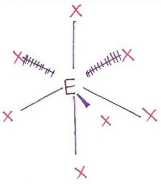
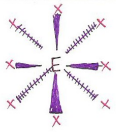
Valence Shell Electron Pair Repulsion (VSPER) theory is used to predict the geometric shape of the molecules based on the electron repulsive force. There are some limitation to VSEPR.

Introduction

The shapes of the molecules is determined mainly by the electrons surrounding the central atom. Therefore, VSEPR theory gives simple directions on how to predict the shape of the molecules. The VSEPR model combines the original ideas of Sidwick and Powell and further development of Nyholm and Gillespie.

How VSEPR works

In a molecule EX_n, the valence shell electron pair around the central atom E and the E-X single bonds are very important due to the repulsion in which determine the shape of the molecule. The repulsions decrease in order of: lone pair-lone pair, lone pair-bonding pair, bonding pair-bonding pair. At the same time, the repulsion would decrease in order of: triple bond-single bond, double bond-single bond, and single bond-single bond if the central atom E has multiple bonds. The difference between the electronegativities of E and X also determine the repulsive force between the bonding pairs. If electron-electron repulsive force is less, then more electron density is drawn away from the central atom E.

Formula EX_n	Coordination number of atom E	Shape	Spatial representation.
EX_2	2	Linear	
EX_3	3	Trigonal planar	
EX_4	4	Tetrahedral	
EX_5	5	Trigonal bipyramidal	
EX_6	6	Octahedral	
EX_7	7	Pentagonal bipyramidal	
EX_8	8	Square antiprismatic	

Shape determination:

VSEPR model works better for simple halides of the p-block elements but can also be used with other substituents. It does not take steric factors, size of the substituents into account. Therefore, the shape of the molecules are arranged so that the energy is minimized. For example:

- BeCl2 has minimum energy when it is a linear molecule.
- BCl3 takes the shape of trigonal planar.

Lone pair electrons are also taken into account. When lone pair electrons are present, the "parent structure" are used as a guideline for determining the shape..

References

1. Li, Kee W., Gong D. zhou, and Thomas Chung W. Mak. *Advanced structural inorganic chemistry*. Oxford, New York: Oxford University Press, 2008. Print.
2. Housecroft, Catherine E., and Alan G. Sharpe. *Inorganic Chemistry Solutions Manual*. 3rd ed. Harlow: Pearson/Prentice Hall, 2008. Print.

Problems

1. What is VSEPR used in chemistry?

It is used to predict the molecular shape of molecules

2. How to predict a molecule structure using VSEPR theory?

First step is to count the total number of valence electrons. After the total number of electrons is determined, this number is divided by two to give the total number of electron pairs. With the electron pairs of the molecule, the shape of the molecule is determined based on the table shown above.

3. What is the shape of PF_5 ?

It is trigonal bipyramidal because it has total of 20 electron pairs. Each Fluorine atom give 1 electron to the Phosphorus central atom which creates total of 5 pairs. Also, each Fluorine atom has 3 electron pairs. With the presence of 5 Fluorine atom, there are 15 more electron pairs so there are 20 electron pairs total.
