

Valence Shell Electron Pair Repulsion Theory

Introduction

The properties of molecules depend not only on the bonding of atoms but also on molecular geometry.

Molecular geometry- is the three dimensional arrangement of a molecule's atoms in space.

The polarity of each bond, along with the geometry of the molecule, determines molecular polarity.

Molecular polarity- is the uneven distribution of molecular charge.

Chemists discuss molecular shapes in terms of two theories:

1. *Valence Shell Electron Pair Repulsion (VSEPR) theory.*
2. *Hybridization theory.*

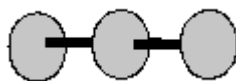
At the most basic level “shape” refers to the spatial disposition of two or more atoms about another atom. The other atom is referred to as the central atom.

Bellow shows five of the most common molecular shapes in organic chemistry;

Structure

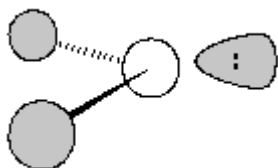
Shape

Example



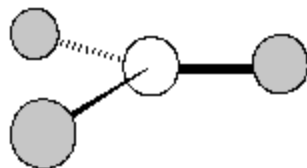
Linear

CO₂



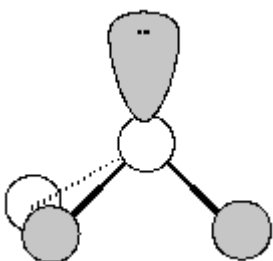
Bent

H₂O

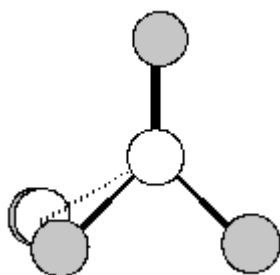


Trigonal Planar

BF₃



Trigonal Pyramidal



Tetrahedral



VSEPR Theory

The abbreviation VSEPR stands for "valence-shell, electron-pair repulsion," referring to the repulsion between pairs of valence electrons of the atoms in a molecule.

Coulomb's Law states "like charges repel". VSEPR theory is merely a restatement of Coulomb's law: areas of electron density will be arrayed around a central atom in such a way to minimize the repulsions between them. Minimizing electron-electron repulsion is achieved by maximizing the distance between the regions of electron density. Maximum distance means maximum angle between bonds. "Area of electron-density" means electron pairs, either bonding or non-bonding.

In case of CO_2 the carbon is double bonded to each oxygen atom. Thus there are two regions of electron density around the carbon, and the repulsion between them is minimized when they are 180° apart i.e. when O-C-O bond angle is 180° .

In contrast, there are four areas of electron density around the oxygen atom in a water molecule, two bonding electron pairs and two non-bonding electron pairs. The best way to minimize the repulsion between four regions of electron density is to distribute them in a tetrahedral array about the central atom.

The tetrahedral bond angle is 109.5° . The H-O-H bond angle in water is 104.5° . The decrease from the tetrahedral value is rationalized by assuming that repulsions between the two non-bonding pairs are greater than those between the two bonding pairs, thus, forcing the bonding pairs to compress slightly in order to allow the non-bonding pairs to get slightly farther apart.

In CH_4 , where the four C-H bonds are identical, the H-C-H angle is 109.5° .

Exercise;

Sign on the web page given; <http://www.inchm.bris.ac.uk/schools/vsepr/index.htm>

Predict the shape of the following molecules BCl_3 .

BCl_3

Click this molecule on the website to be able to see animations and draw the molecule.

1. Decide which is the central atom in a molecule.

In cases of ambiguity, pick the least electronegative atom as this atom will be better able to share its electrons with the other atoms in the molecule.

Ans. _____

2. What is the group number of the central atom?

Ans. _____

3. Count up the valence (outer shell) electrons on the central atom.

Ans. _____

4. Count up the electrons used by the outer atoms to make bonds with the central atom.

Ans. _____

5. The sum of (2) + (3) divided by two gives the Valence Shell Electron Pair (VSEP) count.

Ans. _____

6. The predicted geometry of the molecule is based on the number of VSEP.

VSEP	SHAPE
2	Linear
3	Trigonal Planar
4	Tetrahedral
5	Trigonal Bipyramid
6	Octahedral

Ans. _____

7. Click on the 3-D rotatable diagram to draw the molecule in the space provided;

8. What is the Cl-B-Cl bond angle?

Ans. _____

The following website has a complete table relating structural units, lone pairs, shapes bond angles, structure and examples.

<http://chemistry.jcu.edu/mwaner/GeneralChemistry/VSEPR/VSEPRcomplete.htm>

Hybridization Theory;

If there are two regions of electron density around a central atom, the atom is said to be **sp** hybridized.

If there are three regions of electron density around a central atom, the atom is said to be **sp²** hybridized

If there are four regions of electron density around the central atom, the atom is said to be sp^3 hybridized.

In general, if $s^m p^n$, then the sum of the superscripts is equal to the number of regions of electron density around a central atom.

If $(m+n) = 2$ for a given atom, the shape about the atom is Linear.

If $(m+n) = 3$ for a given atom, the shape is trigonal planar.

If $(m+n) = 4$ the shape is either bent, pyramidal, or tetrahedral depending on the number of atoms attached to the central atom.

Use the link above to answer the following questions;

1. In hydrogen cyanide, HCN, the carbon atom is sp hybridized. The shape of HCN is best described as linear bent trigonal planar pyramidal tetrahedral
2. Beryllium chloride, $BeCl_2$, is a linear molecule. The hybridization of the beryllium atom is best described as sp sp^2 sp^3
3. Which of the following combinations best describes the hybridization and shape of the oxygen atom in methanol, CH_3OH ? sp and linear sp^2 and bent sp^3 and bent sp^3 and pyramidal sp^3 and tetrahedral.

Cooperative Learning Team Activity;

Using the two websites above complete the following table;

Name of shape	Example	Dot structure	Hybrid.	# of bonds	Bond Angle	# unshared electrons	Group # of central atom	Shape
bent	H ₂ O			2		2	16	
tetrahedral	CH ₄			4		0	14	
Trigonal pyramid	NH ₃			3		1	15	
Trigonal planar	BCl ₃			3		0	13	

Notes;

1. Instructions to download Chime are bollow.
2. This tutorial should take around 55 min. Make good time of your time.

Instructions to download Chime.

1. Go to <http://www.umass.edu/microbio/chime/getchime.htm>
2. Click on Register & Download Chime
3. Click on 1. You must register at MDL.
4. Fill out all stared boxes.
5. Check User Status box and Submit Query.
6. Make sure you memorize your user name.
7. An e-mail will send to you that has your password. Don't lose it. You will need the password and the username to log in.
8. Go to www.mdl.com/downloads/index.jsp
9. Register using user name & password.
10. Click on install.
11. Click Chime.
12. Click on Start download on the right side of the page.
14. Chose save to disk.
15. Chose folder to download and save the program to.
16. When download is done, open and follow directions i.e. click next until finished.