GERMANNA ACADEMIC CENTER FOR EXCELLENCE

VSEPR Theory

The valence-shell electron-pair repulsion (VSEPR) model is often used in chemistry to predict the three dimensional arrangement, or the geometry, of molecules. This model predicts the shape of a molecule by taking into account the repulsion between electron pairs. This handout will discuss how to use the VSEPR model to predict electron and molecular geometry.

You can navigate to specific sections of this handout by clicking the links below.

Important Terms: pg. 1

Drawing a Lewis Structure: pg. 2

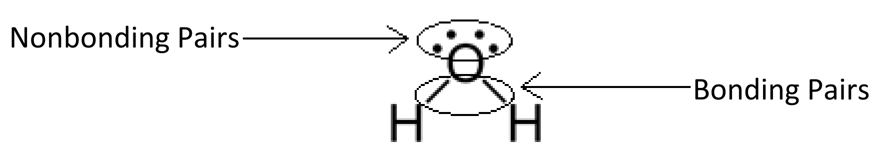
VSEPR Theory Shapes: pg. 3

Practice Problems: pg. 6

Important Terms

Here are some definitions for terms that will be used throughout this handout:

Electron Domain – The region in which electrons are most likely to be found (bonding and nonbonding). A lone pair, single, double, or triple bond represents one region of an electron domain. H_2O has four domains: 2 single bonds and 2 nonbonding lone pairs. Electron Domain may also be referred to as the steric number.



Electron domain geometry - The arrangement of electron domains surrounding the central atom of a molecule or ion.

Molecular geometry - The arrangement of the atoms in a molecule (The nonbonding domains are not included in the description).

Bond angles (BA) - The angle between two adjacent bonds in the same atom. The bond angles are affected by all electron domains, but they only describe the angle between *bonding electrons*.

Lewis structure - A 2-dimensional drawing that shows the bonding of a molecule's atoms as well as lone pairs of electrons that may exist in the molecule.

Octet Rule – Atoms will gain, lose, or share electrons to have a full outer shell consisting of 8 electrons. When drawing Lewis structures or molecules, each atom should have an octet.

Formal Charge – The formal charge can be used to determine the dominant Lewis structure if there is more than one possible configuration. The formal charge of each atom in the molecule should ideally be 0.

Drawing a Lewis Structure

Before the VSEPR theory can be applied, the Lewis structure of the compound must first be drawn. To draw a Lewis structure, follow these steps:

1. Determine the total number of valence electrons (ve^-) by adding the valence electrons from each atom.
2. Choose the central atom. The central atom is typically the least electronegative atom in the molecule and is usually written first in the molecular formula.
3. Arrange the atoms with bonding electrons between all adjacent atoms.
4. Fill in ve^- for outer atoms, so they have octets. There are a few exceptions to the octet rule:

a. Molecules and polyatomic ions with an odd number of valence electrons will not have a full octet. i.e. ClO_2, NO, and NO_2

b. Some molecules will have less than an octet if there are not enough valence electrons or if the formal charges favor the structure without the full octet. This is most often seen with boron and beryllium compounds. Hydrogen will also not have an octet; it can only have two electrons.

c. Hypervalent molecules are formed only on central atoms from period 3 and below on the periodic table. Due to their larger size and the presence of d-orbitals, they can have more than 8 electrons. i.e. PF_5, SF_4

5. If necessary, place any extra ve^- on the central atom.
6. If the central atom does not have an octet, use outer lone pairs to form double or triple bonds.

Example:

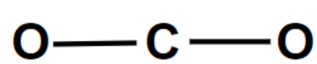
Draw the Lewis structure of CO_2

1. Determine the number of valence electrons.

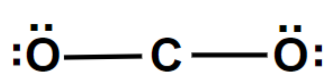
$$1[4\ ve^-]\ (1 \times Carbon) + 2[6\ ve^-]\ (2 \times Oxygen) = 16\ ve^-$$

2. Choose the central atom. Carbon is the least electronegative atom, so it will be in the center.

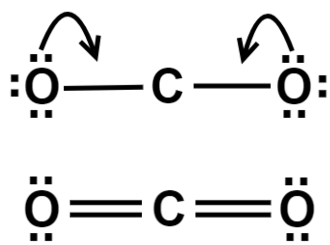
3. Arrange the atoms with bonding electrons.



4. Starting with the outer atoms, fill in valence electrons until the total number of ve^- is reached.



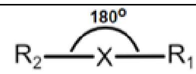
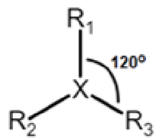
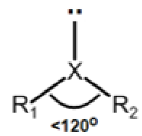
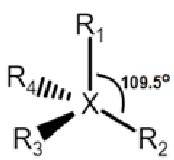
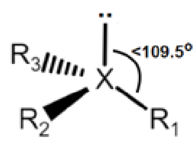
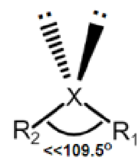
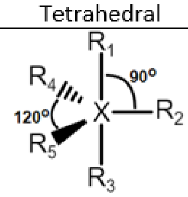
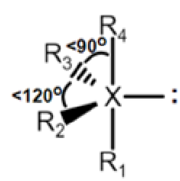
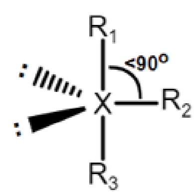
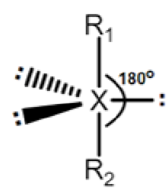
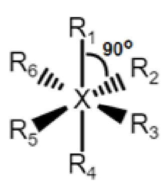
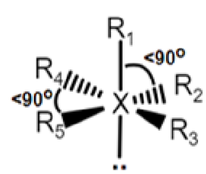
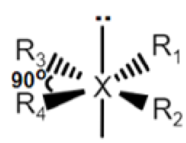
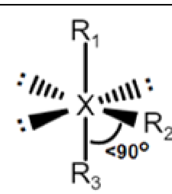
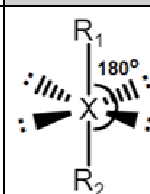
5. There are no extra electrons to place on the central atom.
6. Carbon does not have an octet. Use outer lone pairs to form double bonds.



VSEPR Theory Shapes

To predict the molecular geometry, follow these steps:

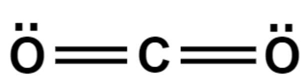
1. Draw the Lewis structure.
2. Count the electron domains, and determine whether they are bonding or non-bonding pairs.
3. Determine the electron domain geometry, molecular geometry, and bond angles. The chart below shows 3-dimensional representations of Lewis structures given the number of bonding and nonbonding pairs within the molecule.

Steric No.	Electron Domain Geometry	Molecular Geometry				
		No Lone Pairs	1 Lone Pair	2 Lone Pair	3 Lone Pair	4 Lone pair
2	Linear	 Linear				
3	Trigonal Planar	 Trigonal planar	 Bent			
4	Tetrahedral	 Tetrahedral	 Trigonal pyramidal	 Bent		
5	Trigonal Bipyramidal	 Trigonal Bipyramidal	 Sawhorse	 T-shaped	 Linear	
6	Octahedral	 Octahedral	 Square pyramidal	 Square planar	 T-shaped	 Linear

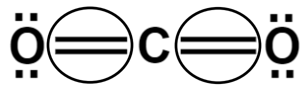
Example:

Predict the electron domain geometry, molecular geometry, and bond angles of carbon dioxide, CO_2.

1.) Draw the Lewis structure.



2.) Count the electron domains, and determine whether they are bonding or non-bonding pairs. CO_2 has 2 electron domains that consist of bonding pairs.



3.) Determine molecular geometry and bonding angles from table.

CO_2 has 2 electron domains, resulting in a linear electron domain geometry. Both electron domains are bonding pairs, so CO_2 has a linear molecular geometry with a bond angle of 180°.

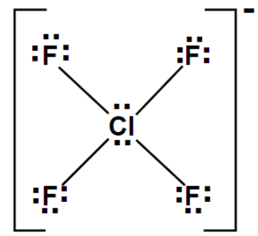
Practice Problems: VSEPR Theory

Predict the electron domain geometry, molecular geometry, and bond angles of the following molecules after drawing valid Lewis structures. Note: some molecules may have more than one central atom.

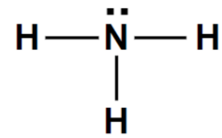
1.) ClF_4^-
2.) NH_3
3.) C_2H_2
4.) SF_4
5.) CH_3COOH

Solutions

1. Electron Domain Geometry: Octahedral
   Molecular Geometry: Square Planar
   Bond Angle: 90°

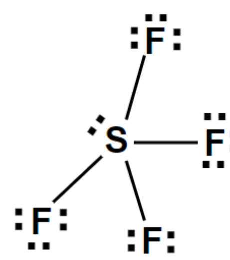


2. Electron Domain Geometry: Tetrahedral
   Molecular Geometry: Trigonal Pyramidal
   Bond Angle: <109.5°



3. Electron Domain Geometry: Linear
   Molecular Geometry: Linear
   Bond Angle: 180°

4. Electron Domain Geometry: Trigonal Bipyramidal
   Molecular Geometry: Sawhorse
   Bond Angle: <90° and <120°.



5. **C_1:** Electron Domain Geometry: Tetrahedral
   Molecular Geometry: Tetrahedral
   Bond Angle: 109.5°
   C_2: Electron Domain Geometry: Trigonal Planar
   Molecular Geometry: Trigonal Planar
   Bond Angle: 120°
   O_3: Electron Domain Geometry: Tetrahedral
   Molecular Geometry: Bent
   Bond Angle: <<109.5°