Chem 103, Section F0F  
Unit VI - Compounds Part II: Covalent Compounds  
Lecture 17

- Using the Valence-Shell Electron-Pair Repulsion (VSEPR) Theory to predict molecular shapes  
- Molecular shape and polarity

Lecture 17 - Covalent Bonding

Reading in Silberberg  
• Chapter 10, Section 2  
  - Valence-Shell Electron-Pair Repulsion (VSEPR) Theory and Molecular Shape  
• Chapter 10, Section 3  
  - Molecular Shape and Molecular Polarity

Lecture 17 - Introduction

In this lecture we will look into predicting molecular shapes and polarity  
• Using a simply theory called the Valence-Shell Electron-Pair Repulsion (VSEPR) Theory it is possible to predict the shape of a molecule starting with its Lewis structure.  
• The molecular structure can then be coupled with electronegativity to predict molecular polarity.  
• Molecular shape and polarity have a marked influence on a molecule's physical properties.  
  - This is particularly the case for biological molecules.

Lecture 17 - VSEPR and Molecular Shape

The main principle of VSEPR is  
• Each group of valence electrons (VSEP) around a central atoms is located as far away as possible from the other groups (R).  

A “group” is any number of electrons that are located near to one another:  
• A non bonded pair of electrons (2 e⁻’s)  
• A single bond (2 e⁻’s)  
• A double bond (4 e⁻’s)  
• A triple bond (6 e⁻’s)  
• A lone free radical electron (1 e⁻)

Lecture 17 - VSEPR and Molecular Shape

Placing the groups as far apart as possible favors a limited set of electron-group geometries.

Lecture 17 - VSEPR and Molecular Shape

Once the electron group geometry is established, the molecular shape is determined by the resulting arrangement of the surrounding atoms about the central atom.
Lecture 17 - VSEPR and Molecular Shape

Two electron-groups (Linear electron-group geometry):

Three electron-groups (Trigonal electron-group geometry):

Lecture 17 - VSEPR and Molecular Shape

Four electron-groups (Tetrahedral electron-group geometry):

Five electron-groups (Trigonal bipyramidal electron-group geometry):

Six electron-groups (Octahedral electron-group geometry):

The 4-step approach to determining molecular shape with VSEPR:

1. Step 1: Write the Lewis structure
2. Step 2: Assign an electron-group arrangement by counting up the electron-groups
3. Step 3: Predict the ideal bond angle from the electron-group arrangement
4. Step 4: Draw and name the molecular shape by counting the bonding groups separately from the nonbonding groups.
Lecture 17 - VSEPR and Molecular Shape

Tutorials and animations
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Lecture 17 - Clicker Question 1
What is the electron group arrangement for SO$_2$?
A) Linear
B) Trigonal planar
C) Tetrahedral
D) Trigonal bipyramidal
E) Octahedral

Lecture 17 - Clicker Question 2
What is the molecular shape for SO$_2$?
A) Linear
B) Trigonal planar
C) Tetrahedral
D) Bent
E) Seesaw

Lecture 17 - Clicker Question 3
What is the ideal O-S-O bond angle?
A) 180°
B) 120°
C) 109.5°
D) 90°
E) 45°

Lecture 17 - Question 4
Determine the electron-group arrangement, molecular shape, and ideal bond angle for N$_2$O (N is central)?

Using formal charges, which resonance structure for N$_2$O is the most probable?

Lecture 17 - VSEPR and Molecular Shape
When molecules have more than one central atom, each is treated separately.
Lecture 17 - Molecular Polarity

Molecules containing polar bonds can exhibit molecular polarity.

- The polarity is measured in units of debyes (D), which is equal to the magnitude of the partial charges times the distance separating them (1 D = 3.34 x 10^-30 C•m).

\[ \delta^+ \quad \delta^- \]

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Lecture 17 - Molecular Polarity

Molecules containing polar bonds can exhibit molecular polarity.

- For diatomic molecules, the molecular dipole is equal to the bond dipole.

\[ \delta^+ \quad \delta^- \]

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Lecture 17 - Molecular Polarity

Molecules containing polar bonds can exhibit molecular polarity.

- For molecules with more than two atoms, both the bond dipoles and the molecular shape must be considered in determining the molecular dipole.

Water has a net dipole moment

Carbon dioxide has no net dipole moment

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Lecture 17 - Molecular Polarity

Dipole moment

- Chloroform (CHCl₃) has a dipole net dipole moment

- Carbon tetrachloride does not have a net dipole moment.

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Lecture 17 - Molecular Polarity

Molecular polarity can have a marked effect on a molecule’s physical properties.

- Polar molecules will align in an electrical field.

Dipole moment and physical properties

- trans-Dichloroethene (C₂H₂Cl₂) has no net dipole moment and a boiling point of 47.5°C.

- cis-Dichloroethene (C₂H₂Cl₂) has a net dipole moment and a boiling point of 60.3°C (13°C higher).

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Lecture 17 - Clicker Question 5

Which molecule has the greater molecular dipole moment?

A) $\text{SO}_2$
B) $\text{SO}_3$

Unit VI - Up Next

Lecture 18 - Theories of Covalent Bonding
- Valence Bond Theory and Orbital Hybridization
- The Mode of Orbital Overlap and the Types of Covalent Bonds.

The End