VESPR Theory

Chapter 4.3

Molecular Geometry

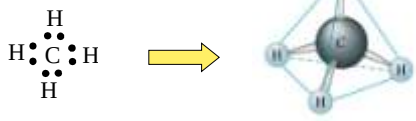
- Critical to know geometry for predictions of structures and the polarity of molecules
- We will start with a method (VESPR theory) for geometry prediction that is based on CORRECT Lewis structures

VESPR Background

- The Lewis Dot Structure approach provided some insight into molecular structure in terms of bonding, but what about geometry?
- Recall that there are two types of electron pairs: bonding and lone.
- Valence Electron Shell Pair Repulsion (VESPR). 3D structure is determined by minimizing repulsion of electron pairs.

VESPR Background (cont.)

- Must consider both bonding and lone pairs in minimizing repulsion.
- Example: CH_4

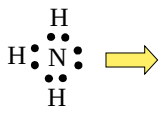


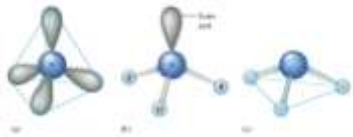
Lewis Structure

VESPR Structure

VESPR Background (cont.)

- Example: NH_3 (both bonding and lone pairs).





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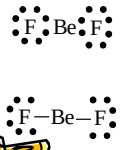
VESPR Structure

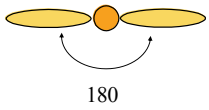
VESPR Applications

- The previous examples illustrate the strategy for applying VESPR to predict molecular structure:
  1. Construct the Lewis Dot Structure
  2. Arranging bonding/lone electron pairs in space such that repulsions are minimized.

VESPR Applications

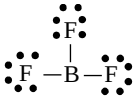
- Linear Structures: angle between bonds is 180
- Example: BeF_2

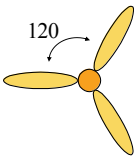




VESPR Applications

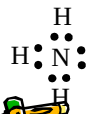
- Trigonal Planar Structures: angle between bonds is 120
- Example: BF_3

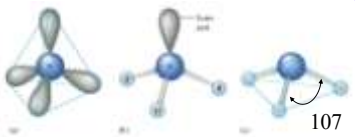




VESPR Applications

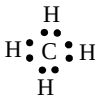
- Pyramidal: Bond angles are <120 , and structure is nonplanar:
- Example: NH_3

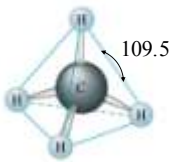




VESPR Applications

- Tetrahedral: angle between bonds is ~109.5
- Example: CH_4





VESPR Applications

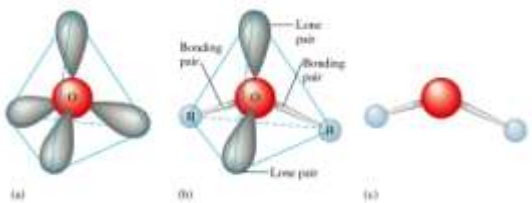
- Tetrahedral: angle may vary from 109.5 exactly due to size differences between bonding and lone pair electron densities

bonding pair

lone pair

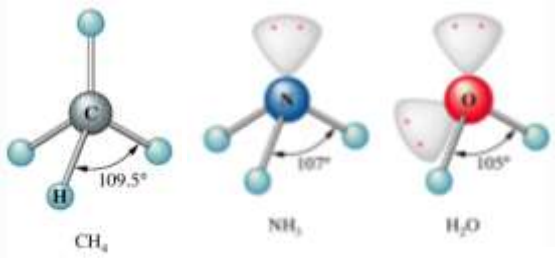
VESPR Applications

- Classic example of tetrahedral angle shift from 109.5 is water:



VESPR Applications

- Comparison of CH_4, NH_3, and H_2O:



Learning Check

Determine the molecular geometry of each of the following:

A. CCl_4

1) tetrahedral 2) pyramidal 3) angular

B. SO_3

1) trigonal planar 2) pyramidal 3) angular

C. PCl_3

1) trigonal planar 2) pyramidal 3) angular

Solution

Determine the molecular geometry of each of the following:

A. CCl_4

1) tetrahedral

B. SO_3

1) trigonal planar

C. PCl_3

2) pyramidal

Popular Shapes