

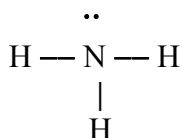
Introduction

This laboratory exercise is intended to reinforce concepts of structure and chemical bonding presented in sections 9.4, 9.5, 9.6, 9.7, 9.8 of your text. You should review and study these sections prior to coming to the laboratory and have the text available for reference as you do the exercise.

VSEPR Theory

As discussed in the text, VSEPR theory provides a reliable process for predicting the molecular geometries of covalent compounds and polyatomic ions from their Lewis structures. The basic premise of the approach is that the electron pairs in the valence shell of an atom minimize mutual repulsions by occupying positions in space as far from one another as possible.

As an example, consider NH_3 which has the Lewis structure shown below.



There are four pairs of electrons in the valence shell of nitrogen, 3 bonding pairs and 1 lone pair. The VSEPR model predicts the four pairs minimize mutual repulsions by adopting a tetrahedral arrangement around the nitrogen atom. This arrangement of all electron pairs about the central atom is referred to as the basic geometry in this exercise. By contrast, the molecular geometry does not include lone pair electrons. Thus the molecular geometry of NH_3 is trigonal pyramidal.

VSEPR theory allows easy prediction of ideal bond angles based on equal repulsions of electron pairs. Thus, the ideal H-N-H angle in NH_3 would be predicted to be 109.5° , the tetrahedral angle. The theory can also be extended to predict the direction of distortion of ideal bond angles resulting from unequal repulsions. For example, it would be surprising if the H-N-H angles in ammonia were all exactly equal to 109.5° . Surely the space requirements of the lone pair and bonding pairs must be different, and hence, the actual H-N-H bond angle must differ somewhat from the tetrahedral value. This is the case as shown in the table below which gives H-A-H bond angles for several molecules with basic geometries which are tetrahedral (A = C or N).

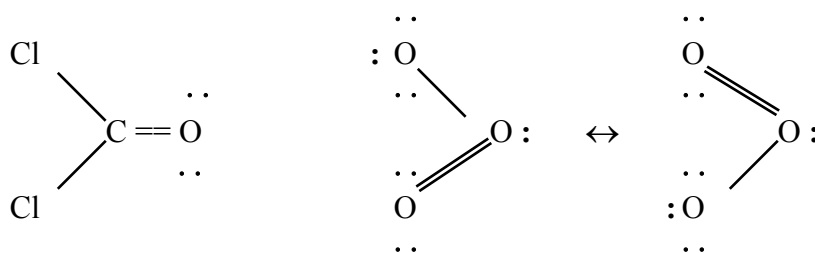
<u>Molecule</u>	<u>H—A—H Angle</u>
CH_4	109.5°
CH_3F	111°
NH_3	107°

Note that only the totally symmetric CH_4 has exactly the tetrahedral bond angle. The H-C-H angle in CH_3F is a few degrees larger than that value while the H-N-H angle of NH_3 is somewhat smaller. The following two VSEPR statements rationalize these observations:

1. The size of a bonding electron pair (and the space it requires) decreases with increasing electronegativity of the ligand (outside atom).
2. A lone pair of electrons is considered to be "bonded to an atom" of zero electronegativity and therefore to require more space than a true bonding pair of electrons.

In CH_3F , the fluorine atom is more electronegative than the hydrogen atoms (see text table). Statement (1) leads us to predict that the C-F bonding pair requires less space than the C-H pairs and that the H-C-H angle should therefore be larger than the ideal tetrahedral angle of 109.5° . Statement (2) suggests the lone pair in NH_3 will "squeeze" the three N-H bonding pairs together to give an observed H-N-H angle less than 109.5° .

A final consideration is the space requirement of double bonds. Based on the Lewis structures below,



both Cl_2CO and O_3 have a basic geometry which is trigonal planar. In Cl_2CO , the Cl-C-Cl angle is 111° while the O-O-O angle in O_3 is 116° , both somewhat less than the 120° expected for a planar triangle. Two conclusions result from these and other similar observations:

1. A true double bond (as in $\text{Cl}_2\text{C}=\text{O}$) has about the same or slightly greater space requirement than a lone pair of electrons.
2. Bonds with an overall bond order between one and two require slightly less space than a lone pair.

Procedure

1. Each group should have/obtain a model kit
2. Be certain your bench area is clean enough to be used as a writing surface.
3. For each substance listed in Parts I and II, do the following:
 - (a) Write the Lewis structure in the space provided under the formula;
 - (b) Construct a 3-dimensional model of the substance using the model kit. Be certain the model is consistent with the Lewis structure and VSEPR theory;
 - (c) Use the model as a guide to fill in the following information in the blanks provided:

Basic Geometry	Molecular Geometry
Ideal Bond Angle	Distortion (Less than, =, more than)
Actual angles (provided by your instructor)	Central Atom Hybridization
4. For each substance that is not an ion determine whether the molecule is non-polar or polar and state so underneath the Lewis structure.

NAME _____

I. Analysis of Molecular Structures**a. Basic Geometry (electron pair)****c. Ideal Bond Angle(s)****e. Actual Angle****b. Molecular Geometry****d. Distortion (<, =, > ideal)****f. Central Atom Hybridization****1. OF₂****a.** _____**c.** _____**e.** _____**b.** _____**d.** _____**f.** _____**2. GeF₂****a.** _____**c.** _____**e.** _____**b.** _____**d.** _____**f.** _____**3. I₃⁻****a.** _____**c.** _____**e.** _____**b.** _____**d.** _____**f.** _____**4. BCl₃****a.** _____**c.** _____**e.** _____**b.** _____**d.** _____**f.** _____**5. NF₃****a.** _____**c.** _____**e.** _____**b.** _____**d.** _____**f.** _____

6. ClF_3

a. _____

b. _____

c. _____

d. _____

e. _____

f. _____

7. NH_4^+

a. _____

b. _____

c. _____

d. _____

e. _____

f. _____

8. ICl_4^-

a. _____

b. _____

c. _____

d. _____

e. _____

f. _____

9. SF_4

a. _____

b. _____

c. _____

d. _____

e. _____

f. _____

10. BrF_5

a. _____

b. _____

c. _____

d. _____

e. _____

f. _____

11. PCl_5

a. _____

b. _____

c. _____

d. _____

e. _____

f. _____

12. AsF_6^-

a. _____

b. _____

c. _____

d. _____

e. _____

f. _____

II Electronegativity and Multiple Bonding Effects

a. Basic Geometry (electron pair)c. Ideal Bond Angle(s)e. Actual Angleb. Molecular Geometryd. Distortion (<, =, > ideal)f. Central Atom Hybridization1. CH₂F₂

a. _____

c. (H-C-H) _____

e. _____

b. _____

d. _____

f. _____

2. (a) F₂CO

a. _____

c. (F-C-F) _____

e. _____

b. _____

d. _____

f. _____

(b) Cl₂CO

a. _____

c. (Cl-C-Cl) _____

e. _____

b. _____

d. _____

f. _____

(c) H₂CO

a. _____

c. (H-C-H) _____

e. _____

b. _____

d. _____

f. _____

Based on the electronegativities of F, Cl and H, which molecule in 2 a, b and c has the largest bond angle? Which has the smallest?

II Electronegativity and Multiple Bonding Effects and Resonance

a. Basic Geometry (electron pair)c. Ideal Bond Angle(s)e. Actual Angleb. Molecular Geometryd. Distortion (<, =, > ideal)f. Central Atom Hybridization3. (a) NO_2^+

a. _____

b. _____

c. _____

d. _____

e. _____

f. _____

(b) NO_2^-

a. _____

b. _____

c. _____

d. _____

e. _____

f. _____

c) NO_3^-

a. _____

b. _____

c. _____

d. _____

e. _____

f. _____

d) NO_2

a. _____

b. _____

c. _____

d. _____

e. _____

f. _____