

# Experiment 13

## Molecular Models on a Computer

### PRE-LABORATORY QUESTIONS

The following preparatory questions should be answered before coming to laboratory. They are intended to introduce you to several ideas that are important to aspects of the experiment. You must complete and turn in your work to your instructor before you will be able to begin the experiment.

**Be sure to bring your textbook with you for this experiment. Material in Chapters 8 and 9 will be very useful for questions you will have while doing this experiment.**

1. Complete the following table:

Formula	Drawing	Lewis structure	# bonding Groups (CA*)	# lone pairs of electrons (CA)
H <sub>2</sub> O				
NO <sub>3</sub> <sup>-</sup>				
HCN				

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\* CA = central atom

## Experiment 13

# Molecular Models on a Computer

### EQUIPMENT NEEDED

Computer  
RasMol Software<sup>1</sup>  
Pdb files<sup>2</sup>

In this experiment you will examine the 3-dimensional molecular geometry of a set of molecules using a molecular viewing program called RasMol. To complete this experiment you will need to load the RasMol application on your computer. The software is at <http://mc2.cchem.berkeley.edu/Rasmol/>. Scroll down to the Downloading RasMol - All versions and select the version you need. Which version depends on whether you are running a PC or a Mac.

You will also need the VSEPR files for this activity. The files you need to download depend on whether you are on a PC or Mac. Go to <http://intro.chem.okstate.edu/AP/2003Norman/Inquiry.html> and select the version you need. Be sure the RasMol application and the VSEPR files are in the same directory/folder. The directory/folder will contain the molecular viewing software called RASWIN.EXE and a folder titled EXP13. Within the EXP13 folder are seven folders beginning with the numbers 1 - 6 and a folder titled Packing & Crystals.

PROCEDURE: (If you have any problems following the instructions consult with your instructor or a student next to you.)

1. Open/launch RASWIN.EXE on your computer. Two windows will appear. The smaller active window titled 'RasMol Molecules' should be moved so that it is not on top of the larger window that is titled 'RasMol Version 2.6'.
2. In the window titled 'RasMol Version 2.6' go to the File menu option and select the Open menu choice. A small dialog box will open revealing a directory listing. You should see an open folder icon titled EXP13. Double click on the EXP13 folder. That will open the EXP13 folder and list the seven folders inside EXP13. Double click on the folder titled 1VSEPR. Within the 1VSEPR directory are the files we will be using in this experiment.

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<sup>1</sup> (<http://mc2.cchem.berkeley.edu/Rasmol/>)

<sup>2</sup> [cheminfo.chem.ou.edu/faculty/mra/mra/home.html](http://cheminfo.chem.ou.edu/faculty/mra/mra/home.html)

## I. VSEPR

- A. In the Folder titled 1VSEPR open the Folder titled 2Family and examine both of the molecules,  $\text{BeF}_2$  and  $\text{CO}_2$ . Complete the table below. View each molecule individually. (Check instructions at the end of the activity.) Before looking at the 2<sup>nd</sup> molecule be sure to Close (menu item under the File Menu) the first molecule.

Draw the molecule (from the RasMol window) and draw the Lewis structure and complete the table with the number of bonding groups of electrons and number of lone pair electrons on the central atom. Measure the bond angle using the 'Angle' tool in the RasMol Molecule window and the bond distance(s). In the table below identify the set of three atoms the bond angle represents and the set of atoms the bond distance represents. Bond angles are in degrees and bond distances are in Angstroms.

Formula	Drawing	Lewis structure	# BG on (CA)	# LP (CA)	Bond Angle(s)	Bond Distance(s)	Molecular Geometry
$\text{BeF}_2$							
$\text{CO}_2$							

- B. Examine all of the molecules in the 3Family Folder. Complete the table below for each molecule.

Formula	Drawing	Lewis structure	# BG on (CA)	# LP (CA)	Bond Angle(s)	Bond Distance(s)	Molecular Geometry
$\text{BF}_3$							
$\text{SO}_3$							
$\text{SO}_2$							

Name \_\_\_\_\_

Section \_\_\_\_\_

How do the nonbonding (lone pair - LP) electrons explain the molecular geometry of  $\text{SO}_2$ ? Explain any differences you notice between the theoretical bond angles and your observed values ( $\text{SO}_2(\text{LP}).\text{pdb}$ ).

C. Examine  $\text{CH}_4$ ,  $\text{NH}_3$  and  $\text{H}_2\text{O}$  molecules in the 4Family directory. Complete the table below.

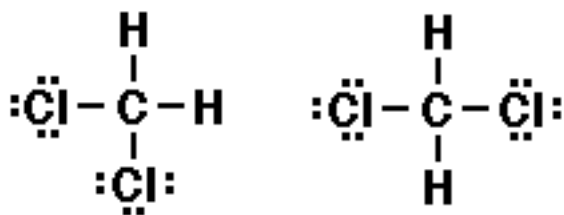
Formula	Drawing	Lewis structure	# BG on (CA)	# LP (CA)	Bond Angle(s)	Bond Distance(s)	Molecular Geometry
$\text{CH}_4$							
$\text{NH}_3$							
$\text{H}_2\text{O}$							

How do the nonbonding (lone pair - LP) electrons explain the molecular geometry of  $\text{NH}_3$  and  $\text{H}_2\text{O}$ ? Explain any differences you notice between the theoretical bond angles and your observed values.

Name \_\_\_\_\_

Section \_\_\_\_\_

Below are two Lewis structures for the compound  $\text{CH}_2\text{Cl}_2$ . Use the file  $\text{CH}_2\text{Cl}_2$ .pdb to determine whether the two structures are the same or different representations. Explain your conclusion.



Look at the three files  $\text{CH}_3\text{F}$ .pdb,  $\text{CH}_3\text{Cl}$ .pdb and  $\text{CH}_3\text{I}$ .pdb. Measure the bond distance for the C–X bond in each. Record your data below, and explain the trend you observe. Estimate the C–Br bond distance in  $\text{CH}_3\text{Br}$ . (Note: You should look at each file using the Spacefill option under the Display Menu.)

Name \_\_\_\_\_

Section \_\_\_\_\_

D. Examine the molecules in the 5Family directory. Complete the table below.

Formula	Drawing	Lewis structure	# BG on (CA)	# LP (CA)	Bond Angle(s)	Bond Distance(s)	Molecular Geometry
PF <sub>5</sub>							
SF <sub>4</sub>							
ClF <sub>3</sub>							
XeF <sub>2</sub>							

How do the nonbonding (lone pair - LP) electrons explain the molecular geometry of SF<sub>4</sub> and ClF<sub>3</sub>? Explain any differences you notice between the theoretical bond angles and your observed values.

Name \_\_\_\_\_

Section \_\_\_\_\_

E. Examine the molecules in the 6Family directory. Complete the table below.

Formula	Drawing	Lewis structure	# BG on (CA)	# LP (CA)	Bond Angle(s)	Bond Distance(s)	Molecular Geometry
SF <sub>6</sub>							
IF <sub>5</sub>							
XeF <sub>4</sub>							

How do the nonbonding (lone pair - LP) electrons explain the molecular geometry of XeF<sub>4</sub> and IF<sub>5</sub>? Explain any differences you notice between the theoretical bond angles and your observed values.

Name \_\_\_\_\_

Section \_\_\_\_\_

F. Complete the following table without the assistance of the RasMol molecular model viewer.

Formula	Drawing	Lewis structure	# bonding Groups	# lone pairs of electrons	Bond Angle (s)	Molecular Geometry
$\text{ClO}_3^-$						
$\text{ICl}_2^-$						
$\text{ClO}_4^-$						
$\text{NO}_2^-$						
$\text{BrF}_3$						



## HELP USING RASMOL

## Menu Choices (Important to us)

## File

Open...opens to the directory containing RASMOL.EXE. So every time you need to open a new pdb file you will have to double-click on EXP13, then double-click on 1VSEPR, then double-click on the 'family' folder you are working in. From the 'family' folder the pdb files will appear in the left portion of the Open dialog box. Double-click on the pdb file you wish to open.

Close...closes the particular pdb file that is selected in the RasMol Molecules Windoid so the molecule in the main viewer window disappears. The maximum number of molecules that will be displayed simultaneously is five.

## Display

Ball & Stick...this will be the display mode of choice for our investigation. You are welcome to investigate the other options in this menu to see how the molecule appears in the molecular viewer window.

Spacefill...this is another mode that is a better view of the relative sizes of the atoms in the molecules. There may be at least one question in this activity that this mode will be useful.

NOTE: The default display mode after opening a pdb file is not very informative. The first thing that should be done is to change the 'Display' to Ball & Stick to better view the molecule.

The remaining menu choices will not be used during this investigation. You are encouraged to explore the other options.

## MOUSE CONTROL

With a pdb file open in the molecular viewer window (the window titled RasMol Version 2.6), and having changed the display to Ball & Stick there are a number of things we will be doing.

To rotate the molecule....click the left mouse button and drag. This rotates the molecule at its current position.

To translate a molecule to a different location in the viewer....click the right button and drag the molecule to the new location.

To change the 'size' of the molecule hold the SHIFT key down, click the left mouse button and drag.

To rotate in the fixed molecular viewer window plane...hold the SHIFT key down, click the right mouse button and drag.

Name \_\_\_\_\_

Section \_\_\_\_\_

## MEASUREMENTS

Bond lengths...Select Distance in the RasMol Molecules window then click on the two atoms of interest. The atoms clicked and the distance in angstroms will appear in the lower portion of the RasMol Molecules window.

Bond Angles... Select Angle in the RasMol Molecules window then click on the three atoms of interest (be sure to use the correct order). The atoms clicked and the bond angle in degrees will appear in the lower portion of the RasMol Molecules window. If three clicks do not produce an angle the software and you may not be in sync. Click the Angle button 'off' and then 'on' again and repeat by selecting the three atoms.