

# Molecular Modeling

## Introduction to Molecular Modeling

In the following laboratory activities you will examine three-dimensional models of molecules using the computer-based molecular viewing program called Jmol. You can access a version of Jmol for use with these activities at <http://www.chemeddl.org/resources/models360/models.php>.

### Instructions

After obtaining access to the Jmol program you should see an image on your computer screen that looks similar to Figure I. NOTE: The molecule that appears in molecular frame may be different than what is pictured below.

The screenshot shows the ChemEd DL Models 360 web interface. At the top left is the ChemEd DL logo (Chemical Education Digital Library). To the right is a search bar labeled "Find: Name / Formula" with buttons for "Advanced Search", "About", and "Help". Below the search bar are tabs for "Molecules" and "Solids". A secondary navigation bar contains tabs for "3D structure: Jmol", "Molecular Properties", "Images", and "Export". The main content area is titled "Beryllium Chloride BeCl<sub>2</sub>". On the left is a 3D ball-and-stick model of the molecule, showing a central grey sphere (Be) bonded to two green spheres (Cl). To the right of the model is a "Display" control panel with several checkboxes: "Spin Molecule", "VdW radii", "Bond Length", "Bond Angles", "Atom Labels", "Partial charges", "Labels off", "Molecular Dipole", and "Bond Dipoles". Below this panel are buttons for "Molecular Electrostatic Potential (MEP)", "Molecular Vibrations", "Symmetry Elements for Point Group D=h", and "Molecular Orbitals". On the far right is a "Related Molecules" section with navigation arrows and a list of molecules: ClO<sub>2</sub>(r) Chlorine Dioxide, ClO<sub>2</sub><sup>+</sup> Chlorine Dioxide cation, B<sub>2</sub>H<sub>6</sub> Diborane, N<sub>2</sub>O<sub>4</sub> Dinitrogen Tetraoxide, and H<sub>2</sub>O<sub>2</sub> Hydrogen Peroxide. At the bottom of the interface are three buttons: "Popup window", "Take a picture", and "Reset".

Figure 1.

\* Jmol is a free, open source molecule viewer for students, educators, and researchers in chemistry and biochemistry. It is cross-platform, running on Windows, Mac OS X, and Linux/Unix systems (see: <http://jmol.sourceforge.net/>). A team of researchers are updating and improving the program on a constant basis. Robert Hanson of St. Olaf College has been particularly helpful to the authors of these activities.

In the activity that follows, formulas for specific compounds must be entered into the Find Name/Formula cell near the top of the Models 360 web page. As you enter the formula a dropdown list of possible choices will appear. Select the compound you are interested in viewing. This will initiate the process of loading the molecular model of the compound. Throughout the activity measuring bond lengths and/or bond angles will be required.

**To measure a bond length:** hold the cursor over an atom. Double click on the atom. As you move the cursor to another atom a colored dotted line should appear. When you place the cursor over a second atom, double click on it. The colored line should change color and a value for the length should appear. Jmol seems to be a little sensitive to this operation so you might have to try this several times. It may also be necessary to rotate the molecule to see the bond length clearly.

**To measure a bond angle:** double click on one of the end atoms. Then drag the cursor to the middle atom in the angle. Single click on this atom, then move the cursor to the other end atom and double click. The angle in degrees should appear as the dotted line changes color. It may also be necessary to rotate the molecule to see the bond angle clearly.

**To rotate the molecule,** click anywhere in the window and drag your mouse around. You can rotate the molecule in the plane of the screen and resize it by using the shift key when you click/drag the mouse side by side or up and down.

## I. VSEPR\*

Name \_\_\_\_\_

Section \_\_\_\_\_

It may be helpful for you to refer to the table of molecular geometries found in most general chemistry textbooks. In Tro there are tables found on page 434 (following pages 426 – 433)

A. Using Jmol, examine  $\text{BeCl}_2$  and  $\text{CO}_2$ . (Enter each formula into the Find Name/Formula cell near the top of the Models 360 web page.) Write the molecular formula for each molecule in the space below. Draw and label the molecules and measure and record their bond angles.

B. Using Jmol, examine  $\text{BF}_3$  and  $\text{SO}_2$ . Write the molecular formula for each molecule in the space below. Draw and label these molecules and measure and record their bond angles. Draw the Lewis structure for each molecule. Why is  $\text{SO}_2$  shaped like it is and not linear? How is it different from the molecules in section A? What is similar about all of the molecules in List B? Describe any difference between the angles you measure and the theoretical ones (see page 434 in your textbook to see what the theoretically expected angles should be).

C. Repeat step B for  $\text{CH}_4$ ,  $\text{NH}_3$  and  $\text{H}_2\text{O}$  (i.e., open them, measure their bond angles, and draw the Lewis structures). Write the molecular formula for each molecule. What is similar about all of the molecules in List C? Compare the actual bond angles with the theoretically expected angles (look at page 434 in your textbook). Explain any trend in bond angles that you observe.

D. All of the molecules  $\text{PF}_5$ ,  $\text{SF}_4$ ,  $\text{ClF}_3$  and  $\text{I}_3^-$  have five regions/domains of electron density around the central atom. Open the  $\text{PF}_5$  molecule, and examine the two different F-P-F angles in the molecule. Draw and label this molecule. Predict where the lone pairs (nonbonding domains) will go in molecules that have one, two, and three lone pairs (nonbonding domains). Now, open the other files, write the molecular formula for each molecule, measure their bond angles, and draw the molecules. Were your predictions correct? At what locations do the lone pairs go in five-coordinate molecules?

E. Using Jmol, examine SF<sub>6</sub>, F<sub>5</sub>I, and F<sub>4</sub>Xe, all of which have six regions/domains of electron density. Write the molecular formula for each molecule. Draw the molecules and measure their bond angles. Draw the Lewis structure for each molecule. How do nonbonding (lone pair—LP) electrons explain the molecular geometries of F<sub>4</sub>Xe and F<sub>5</sub>I? Explain any differences you notice between the theoretically expected bond angles and your observed values.

## II. CARBON COMPOUNDS

Name \_\_\_\_\_

Section \_\_\_\_\_

### A. Bond Types

In Jmol, open (CH<sub>3</sub>CH<sub>3</sub>), double (CH<sub>2</sub>CH<sub>2</sub>), and triple (HCCH). Measure and record the carbon-to-carbon bond lengths for single (CH<sub>3</sub>CH<sub>3</sub>), double (CH<sub>2</sub>CH<sub>2</sub>), and triple (HCCH) bonds. Make a generalization comparing the lengths of single, double, and triple bonds. Propose a reason for your generalization.

### III. PERIODIC TRENDS

Name \_\_\_\_\_

Section \_\_\_\_\_

For this portion of the activity you will use the following links to Jmol molecular models of ONF, ONCl, ONBr and ONI that are located at St. Olaf College.

The four nitrosyl halides;

ONF (<https://chemapps.stolaf.edu/jmol/jmol.php?model=FN%3DO>)

ONCl (<https://chemapps.stolaf.edu/jmol/jmol.php?model=CIN%3DO>)

ONBr (<https://chemapps.stolaf.edu/jmol/jmol.php?model=BrN%3DO>)

ONI (<https://chemapps.stolaf.edu/jmol/jmol.php?model=IN%3DO>)

A. Draw the Lewis structures for the molecules ONBr, ONCl, ONF, and ONI. Predict the molecular geometries and bond angles for each molecule.

B. In Jmol, examine the four molecules. Draw and label the molecules and measure and record their bond lengths and bond angles.

C. Identify any trends you observe in the measurements you recorded. How are these trends related to the periodic table and to electron configurations? Explain why these trends exist.

D. Draw the Lewis structures for the molecules  $\text{CH}_3\text{F}$ ,  $\text{CH}_3\text{CH}_3$ ,  $\text{CH}_3\text{OH}$ , and  $\text{CH}_3\text{NH}_2$ . Predict the molecular geometries and bond angles for each molecule.



E. In Jmol, examine the four molecules in III.D. Draw and label the molecules and measure and record their bond lengths and bond angles.

F. Identify any trends you observe in the measurements you recorded. How are these trends related to the periodic table and to electron configurations? Explain why these trends exist.