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.

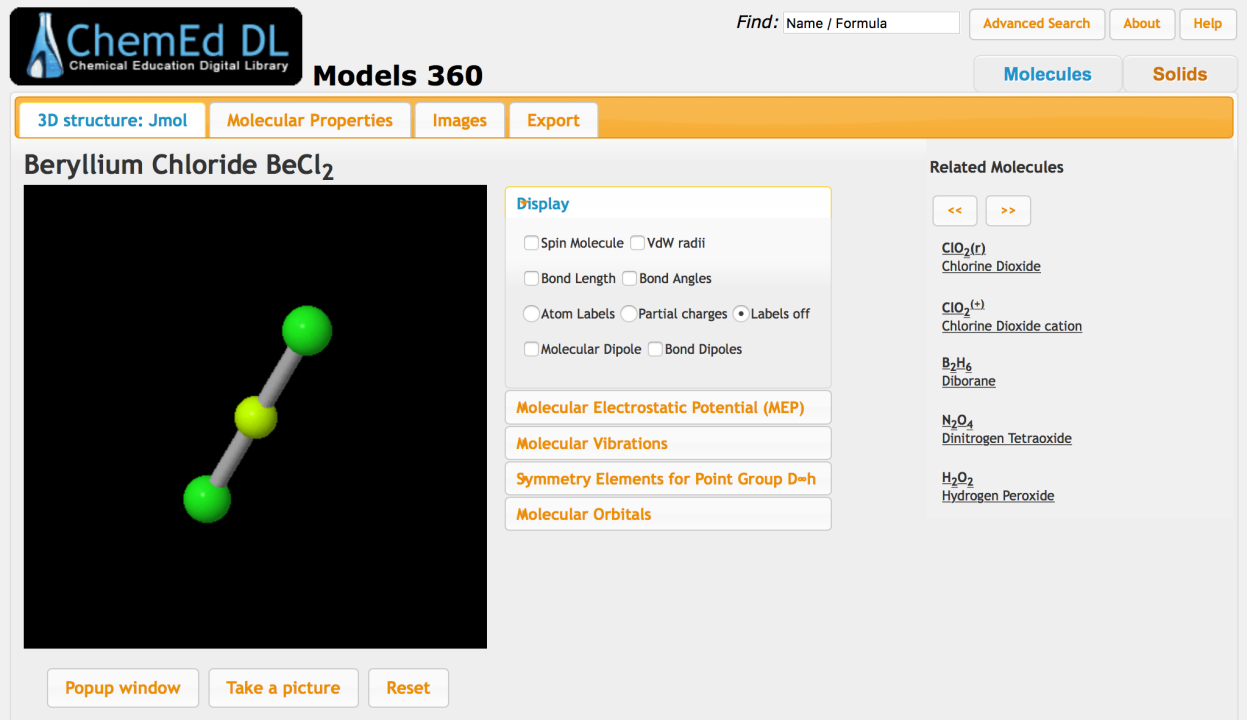


Figure 1.

* 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.

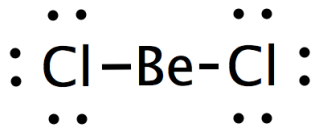
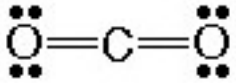
To rotate the molecule, click anywhere in the window and drag your mouse around. You can rotate the molecule in the plane of the screen and resize it by using the shift key when you click/drag the mouse side by side or up and down.

I. VSEPR*

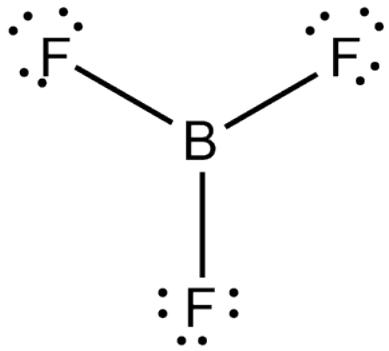
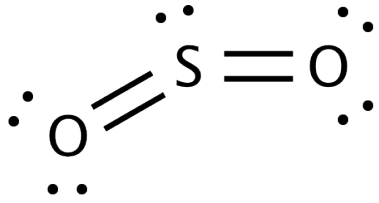
Name _____ Section_____

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 $BeCl_2$ and 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.

	
Cl–Be–Cl bond angle is 180 ˚	O–C–O bond angle is 180 ˚

B. Using Jmol, examine BF_3 and 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 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 bond angles you measure and the theoretical ones (see page 434 in your textbook to see what the theoretically expected angles should be).

	
F–B–F bond angle is 120 ˚	O–S–O bond angle is less than 120 ˚

In SO_2 the sulfur atom has a nonbonding domain of electrons, while in CO_2 there are no nonbonding domains. The nonbonding domain of electrons and the two bonding domains of electrons result in a different molecular geometry (trigonal planar).

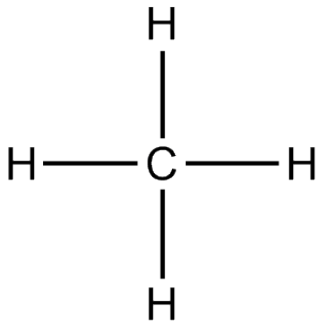
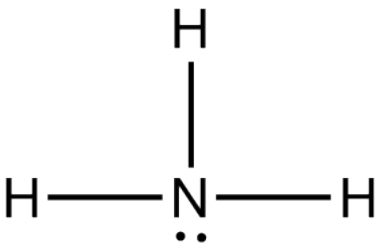
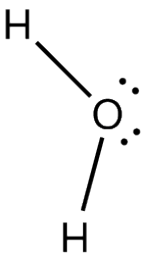
What is similar about all of the molecules in List B?

Both BF_3 and SO_2 have three domains of electrons around the central atom.

Describe any difference between the bond angles you measure and the theoretical ones.

Possibly expect the bond angles to be the same in these two structures, however, SO_2 has a nonbonding domain of electrons, which occupies a larger volume of space resulting in greater lone pair (LP)-bonding pair (BP) repulsions.

C. Repeat step B for CH_4, NH_3 and H_2O (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.

		
H–C–H bond angle is 109.5 ˚	H–N–H bond angle is less than 109.5 ˚	H–O–H bond angle is less than 109.5 ˚

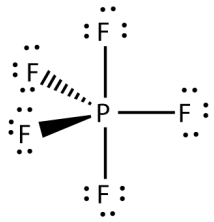
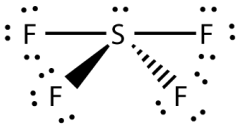
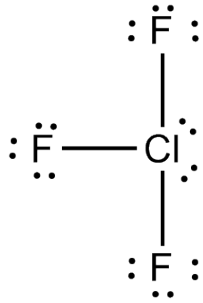
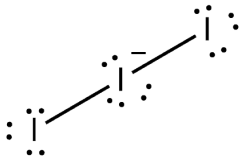
What is similar about all of the molecules in List C?

CH_4, NH_3 and H_2O all have four domains of electrons around the central atom.

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.

The Bond angle in NH_3 and H_2O is less than the ideal bond angle due to lone pair(s) of electrons on the central atom. Because LP-BP repulsions are greater than BP-BP repulsions the bond angles NH_3 and H_2O are less than 109.5˚.

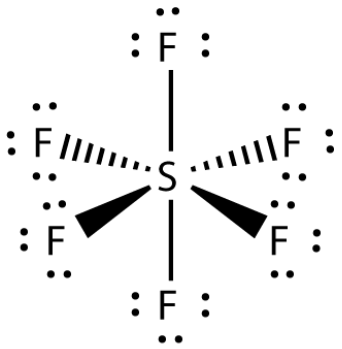
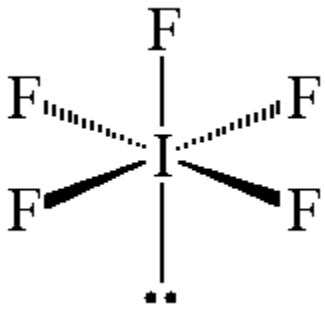
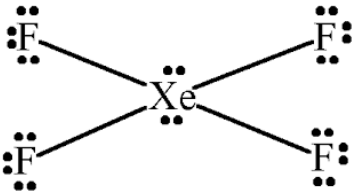
D. All of the molecules PF_5, SF_4, ClF_3 and I_3^- have five regions/domains of electron density around the central atom. Open the PF_5 molecule, and examine the two different F-P-F angles in the molecule. Draw and label this molecule. Predict where the lone pairs (nonbonding domains) will go in molecules 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?

			
F–P–F bond angles are 90 ˚, 120˚ and 180˚	F–S–F bond angles are 90 ˚, 120˚ and 180˚	F–Cl–F bond angles are 90 ˚, and 180˚	I–I–I bond angle is 180˚

Predict where the lone pairs (nonbonding domains) will go in molecules that have one, two, and three lone pairs (nonbonding domains).

When replacing one, two or three bonding pairs with nonbonding domains it is the equatorial terminal atoms that are replaced with lone pair electrons. This is because LP-BP repulsions are reduced when nonbonding domains are in the equatorial positions rather than the axial positions.

E. Using Jmol, examine SF_6, F_5I, and F_4Xe, 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_4Xe and F_5I? Explain any differences you notice between the theoretically expected bond angles and your observed values.

		
F–S–F bond angles are 90 ˚ and 180˚	F–I–F bond angles are 90 ˚ and 180˚	F–Xe–F bond angles are 90 ˚ and 180˚

How do nonbonding (lone pair—LP) electrons explain the molecular geometries of F_4Xe and F_5I? **It makes no difference which bonding pair of electrons is replaced with a nonbonding pair, the resulting square pyramidal molecular geometry is the same for F_5I. However in the case of F_4Xe the nonbonding pairs must go 180 ˚ apart to reduce the LP-BP repulsions.**

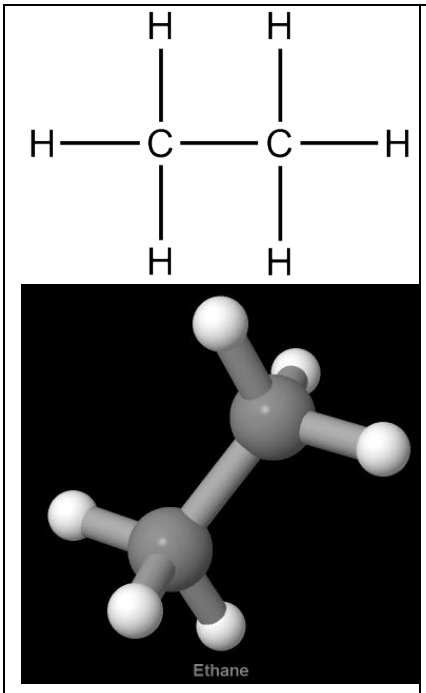
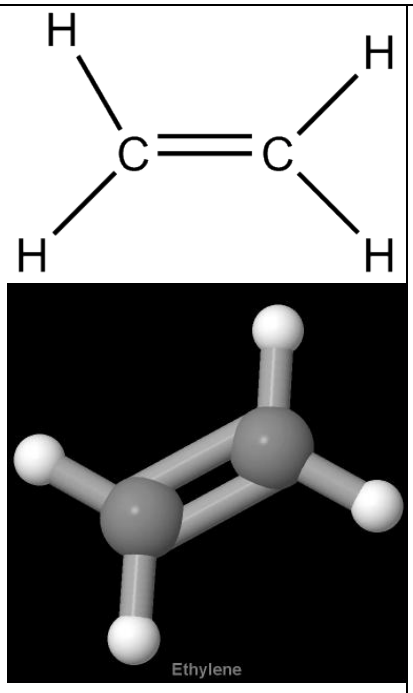
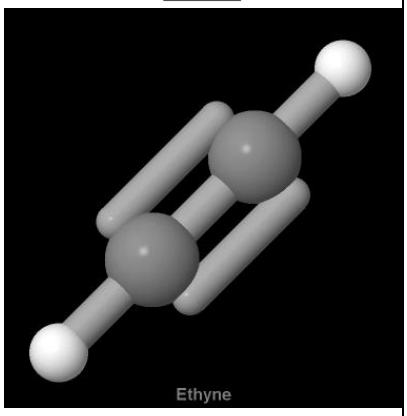
Explain any differences you notice between the theoretically expected bond angles and your observed values. **The differences are due to the lone pair electrons and the fact that LP-BP repulsions are greater compared to BP-BP repulsions.**

II. CARBON COMPOUNDS

Name _____ Section_____

A. Bond Types

In Jmol, open (CH_3CH_3), double (CH_2CH_2), and triple (HCCH). Measure and record the carbon-to-carbon bond lengths for single (CH_3CH_3), double (CH_2CH_2), and triple (HCCH) bonds. Make a generalization comparing the lengths of single, double, and triple bonds. Propose a reason for your generalization.

		
C-C bond distance is 0.153 nm	C-C bond distance is 0.133 nm	C-C bond distance is 0.12 nm

The C-C bond distance decreases from single bond (CH_3CH_3), double bond (CH_2CH_2), and triple bond(HCCH). With more electrons there are greater attractions to the central carbon atoms.

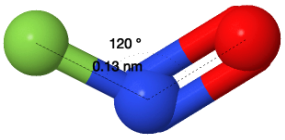
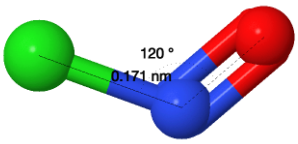
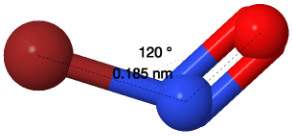
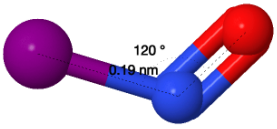
III. PERIODIC TRENDS

Name _____ Section_____

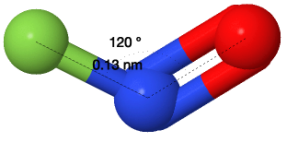
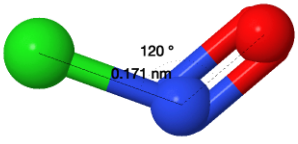
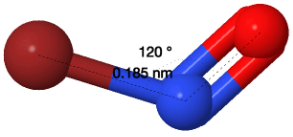
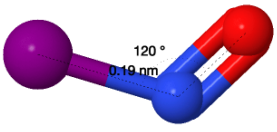
For this portion of the activity you will use the following links to Jmol molecular models of ONF, ONCl, ONBr and ONI that are located at St. Olaf College.
The four nitrosyl halides;

ONF (https://chemapps.stolaf.edu/jmol/jmol.php?model=FN%3DO
ONCl (https://chemapps.stolaf.edu/jmol/jmol.php?model=ClN%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.

			
N-F bond distance is 0.13 nm, the O-N-F bond angle is 120 ˚.	**N-Cl bond distance is 0.171 nm, the O-N-Cl bond angle is 120 ˚.**	**N-Br bond distance is 0.185 nm, the O-N-Br bond angle is 120 ˚.**	**N-I bond distance is 0.190 nm, the O-N-I bond angle is 120 ˚.**
Bent molecular geometry	**Bent molecular geometry**	**Bent molecular geometry**	**Bent molecular geometry**

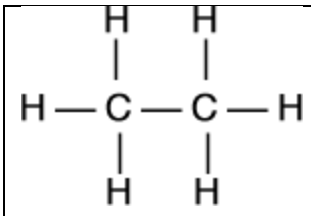
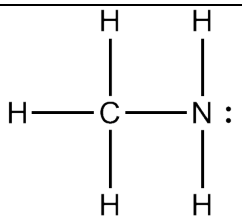
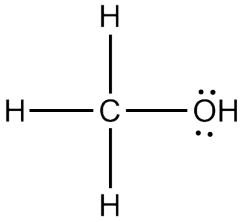
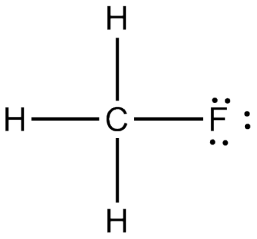
B. In Jmol, examine the four molecules. Draw and label the molecules and measure and record their bond lengths and bond angles.

			
N-F bond distance is 0.13 nm, the O-N-F bond angle is 120 ˚.	**N-Cl bond distance is 0.171 nm, the O-N-Cl bond angle is 120 ˚.**	**N-Br bond distance is 0.185 nm, the O-N-Br bond angle is 120 ˚.**	**N-I bond distance is 0.190 nm, the O-N-I bond angle is 120 ˚.**

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.

There is a trend in the N-X bond distance. As the halogen atom atomic radius gets larger (going from F to Cl to Br to I) the N-X bond distances get larger. Clearly the larger the atom sharing electrons with the nitrogen atom the larger the N-X bond distance.

D. Draw the Lewis structures for the molecules CH_3F, CH_3CH_3, CH_3OH, and CH_3NH_2. Predict the molecular geometries and bond angles for each molecule.

			
C–C bond distance is 0.153 nm	C–O bond distance is 0. 146	C–N bond distance is 0. 142 nm	C–F bond distance is 0.138 nm
The H-C-H bond angles are 107.5˚. The C-C-H bond angle is 111.4˚	The H-O-C bond angle is 107.6 ˚ and the H-C-O bond angle is 106.7˚.	The H-N-C bond angle is 109.6 ˚ and the H-C-N bond angle is 109.1˚.	H-C-F bond angle is 109.6˚ H-C-H bond is 109.3 ˚

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.

The C-X bond distance (X = C, N, O F) gets shorter as the atoms, C, N, O and F move from left to right across the periodic table. This can be understood in terms of the atomic radius of C, N, O and F. Each of these atoms have valence electrons in the 2nd shell (valence shell), and the nuclear charge increases from C, N, O to F. The increase in nuclear charge, coupled with the valence electrons in the same shell results in the valence electrons experiencing a stronger attraction to the nucleus moving from left to right. The stronger the attraction experienced by the valence electrons the smaller the atomic radius of the X atom and the shorter the C-X bond distance becomes.