

BOND LENGTH WITH HYPERCHEM LITE

LAB MOD2.COMP

From Gannon University SIM

INTRODUCTION

The electron cloud surrounding the nucleus of the atom determines the size of the atom. Since this distance is somewhat fuzzy, the atomic radius of an atom is used to measure the size of the atom.

Bond length is the distance between two bonded atoms or the sum of the radii of the two bonded atoms. Bond lengths are usually measured in angstroms, Å ($1 \text{ Å} = 10^{-10} \text{ m}$), or picometers, pm ($1 \text{ pm} = 10^{-12} \text{ m}$).

HyperChem Lite is a molecular modeling and simulation program that uses a computer and CD-ROM based software to predict physical and chemical properties of molecules. This software allows covalent bonds to be considered as if they were springs connecting atoms.

PURPOSE

The purpose of this experiment is to learn to measure bond length and to examine the impact of multiple bonds on bond length.

EQUIPMENT/MATERIALS

Laptop computer with HyperChem Lite installed

Wireless Printer and Paper

HyperChem Lite CD

SAFETY

- Keep goggles on hand for use when dealing with glass, chemicals and/or fire.

PROCEDURE

The HyperChem Lite Window


1. To start HyperChem Lite, put cursor in the HyperChem Lite Icon, then double click on left mouse. The HyperChem Lite window will open the following list of features:
 - a. Menu Bar: contains the different HyperChem Lite menus which include: File, Edit, Build, Display, Set-up, Compute, Cancel and Help.
 - b. Tool Bar: the left side of the screen contains the tools to draw, select, display and move atoms and molecules.
 - c. Workspace: displays current atoms or molecules.
 - d. Status Line: show a brief description of menu item selected and information about drawing.
 - e. Title Bar: shows name of file working on.
 - f. Control Menu Button: contains commands to move, resize, maximize, and close HyperChem Lite windows. It also contains the switch command, which lets you activate other windows.

Measuring Bond Length

Carbon-Nitrogen Bonds

Target molecules: HCN, CH₂NH and CH₃NH₂

To build HCN, CH₂NH and CH₃NH₂, follow these steps:


1. *Left-double click* on the draw icon (). The element table dialog box will appear. *Left-double click* on carbon (C) in the periodic table.
2. *Left click* in the workspace. A carbon atom will appear in the workspace.
3. *Left-double click* on the draw icon. The element table dialog box will appear. *Left-double click* on nitrogen (N) in the periodic table.
4. *Left click* in the workspace. A nitrogen atom will appear in the workspace.
5. *Left click* on carbon and drag cursor to N once to draw a single bond, twice for a double bond and three times for a triple bond, depending on structure being built.
6. *Left click* on Build. *Left click* on Add Hydrogens. A complete molecule will appear. *Left click* on Display. *Left click* on Renderings. Select balls and cylinders, shaded and highlighted. *Left click* OK.
7. Under Setup, *Left click* on molecular mechanics
8. Select Compute. *Left click* on Geometry Optimization. Select Polak-Ribiere. *Left click* OK. The molecule model is now complete and geometrically correct.

9. To measure the bond length. *Left click* on Selection Tool. *Left click* on carbon and drag cursor to nitrogen. The bond length will appear on the lower left below the workspace.
10. Record bond length for the C-N bond, in Angstroms, on the Data Sheet.
11. Clear the molecule by *left clicking* in an open area of the workspace. All the atoms will turn green. Select Edit and *left click* on clear. Select yes to remove the previous molecule.
12. Repeat steps 1-9 to build other C-N molecules. Record bond length. Clear molecule.

Oxygen-Oxygen Bonds

Target molecules: H₂O₂, O₂ and O₃

To build H₂O₂, O₂ and O₃, follow these steps:



1. *Left-double click* on the draw icon (). The element table dialog box will appear. *Left-double click* on oxygen (O) in the periodic table.
2. *Left click* two times in the workspace. Two oxygen atoms will appear in the workspace.
3. Click and drag to form a single bond between the two oxygen atoms.
4. *Left click* Build. *Left click* on Add Hydrogens. A complete molecule will appear.
5. *Left click* on Display. *Left click* on Renderings. Select balls and cylinders, shaded and highlighted. *Left click* OK.
6. Under Setup, *left click* on molecular mechanics.
7. Select Compute, *left click* on Geometry Optimization. Select Polak-Ribiere. *Left click* OK. H₂O₂ molecule model is now complete and geometrically correct.
8. To measure the bond length. *Left click* on Selection Tool. *Left click* on one oxygen and drag cursor to the other oxygen. The bond length will appear on the lower left below the workspace.
9. Record bond length for the O-O bond, in Angstroms, on the Data Sheet.
10. Clear the molecule by *left clicking* in an open area of the workspace. All the atoms will turn green. Select Edit and *left click* on clear. Select yes to remove the previous molecule.

11. Repeat steps 1-3 for the next target molecule, drawing in double or triple bonds. Omit step 4 since the molecule does not contain hydrogen.
12. Continue with steps 5-10 above.

Carbon-Oxygen Bonds

Target molecules: HCOOH, CO, and CO₂


To build HCOOH, CO, and CO₂, follow these steps:

1. *Left-double click* on the drawing icon (). The element table dialog box will appear. *Left-double click* on oxygen (O) in the periodic table. *Left click* twice in the workspace. Two oxygen atoms will appear in the workspace.
2. *Left-double click* on the draw icon (). The element table dialog box will appear. *Left-double click* on carbon (C) in the periodic table.
3. *Left click* in the workspace. A carbon atom will appear in the workspace.
4. *Left click* on carbon and drag cursor to one oxygen to draw a single bond, *Left click* and drag cursor to other oxygen twice for a double bond.
5. *Left click* Build. *Left click* on Add Hydrogens. A complete molecule will appear.
6. *Left click* on Display. *Left click* on Renderings. Select balls and cylinders, shaded and highlighted. *Left click* OK.
7. Under Setup, *left click* on molecular mechanics.
8. Select Compute, *left click* on Geometry Optimization. Select Polak-Ribiere. *Left click* OK. HCOOH molecule model is now complete and geometrically correct.
9. Measure the bond length. *Left click* on Selection Tool. *Left click* on carbon and drag cursor to oxygen. The bond length will appear on the lower left below the workspace.
10. Record bond length and clear molecule.
11. Repeat steps 1-10 to build CO and CO₂, omitting step 5 and adjusting the number of oxygen atoms as needed.

Carbon-Carbon Bonds

Target molecules: C₂H₆, C₂H₄, and C₂H₂

To build C₂H₆, C₂H₄, and C₂H₂, follow these steps:

1. *Left-double click* on the draw icon (). The element table dialog box will appear. *Left-double click* on Carbon (C) in the periodic table. L-click in the workspace twice. Two carbon atoms will appear.
2. *Left click* on one carbon and drag to next once to build a single bond, twice for a double bond and three times for a triple bond.
3. *Left click* Build. *Left click* on Add Hydrogens. A complete molecule will appear.
4. Select Compute, *Left click* on Geometry Optimization. Select Polak-Ribiere. *Left click* OK. C₂H₆ molecule model is now complete and geometrically correct.
5. *Left click* on Display. *Left click* on Renderings. Select Balls and cylinders, Option, shade and highlighted. *Left click* OK.
6. To measure the bond length. *Left click* on Selection Tool. *Left click* on one carbon and drag cursor to the other carbon. The bond length will appear on the lower left below the workspace.
7. Record bond length for the C-C bond, in Angstroms, on the Data Sheet.
8. Clear the molecule by *left clicking* in an open area of the workspace. All the atoms will turn green. Select Edit and *left click* on clear. Select yes to remove the previous molecule.

DATA SHEET

Name _____

Name _____

Period _____ Class _____

Date _____

BOND LENGTH WITH HYPERCHEM LITE

DATA

A. Bond distance for Carbon-Nitrogen bonds:

HCN _____A

CH₂NH _____A

CH₃NH₂ _____A

B. Bond distance for group Oxygen-Oxygen bonds:

H₂O₂ _____A

O₂ _____A

O₃ _____A

C. Bond distance for Carbon-Oxygen bonds:

CO _____A

CO₂ _____A

HCOOH _____A

D. Bond distance for Carbon-Carbon bonds:

C₂H₆ _____A

C₂H₄ _____A

C₂H₂ _____A

EXTENSION: POLARITY AND MOLECULAR SHAPE

Underlined molecules can be found already built in the HyperChem Lite sample file. To access file *left click* on File, *left click* Open, *left-double click* Samples, *left-double click* Vsepr. Structure is already built and geometrically optimized.

To Measure bond Angle:

1. *Left click* on Selection Tool.
2. *Left click* on one atom and drag cursor to other atom. The bond angle will appear on the lower left below the workspace.

FORMULA	BOND ANGLE	SHAPE	POLAR (YES/NO)
BeCl ₂			
<u>BF₃</u>			
SO ₂			
CH ₄			
NH ₃			
SCl ₂			
<u>PF₅</u>			
Second angle for <u>PF₅</u>			
<u>SF₄</u>			
<u>ICl₃</u>			
<u>I₃</u>			
<u>SF₆</u>			
<u>IF₅</u>			
<u>XeF₄</u>			