NAME: _____ Lab Day/Time: _____

Molecular Modeling

BV 1/2009

Purpose

The purposes of this experiment are:

To learn how to use molecular modeling software, a commonly used tool in the chemical and pharmaceutical industry.

To examine the structures of a number of simple molecules to search for common factors affecting molecular structure.

Procedure

There are a variety of software programs available to perform molecular modeling experiments, with names such as Spartan, Mopac, and Gaussian. The one we use is CAChe, and we have a "site license" for it. This means that, although a single copy costs upwards of $1,000, each of you can install a copy on your own computer and use it at will.

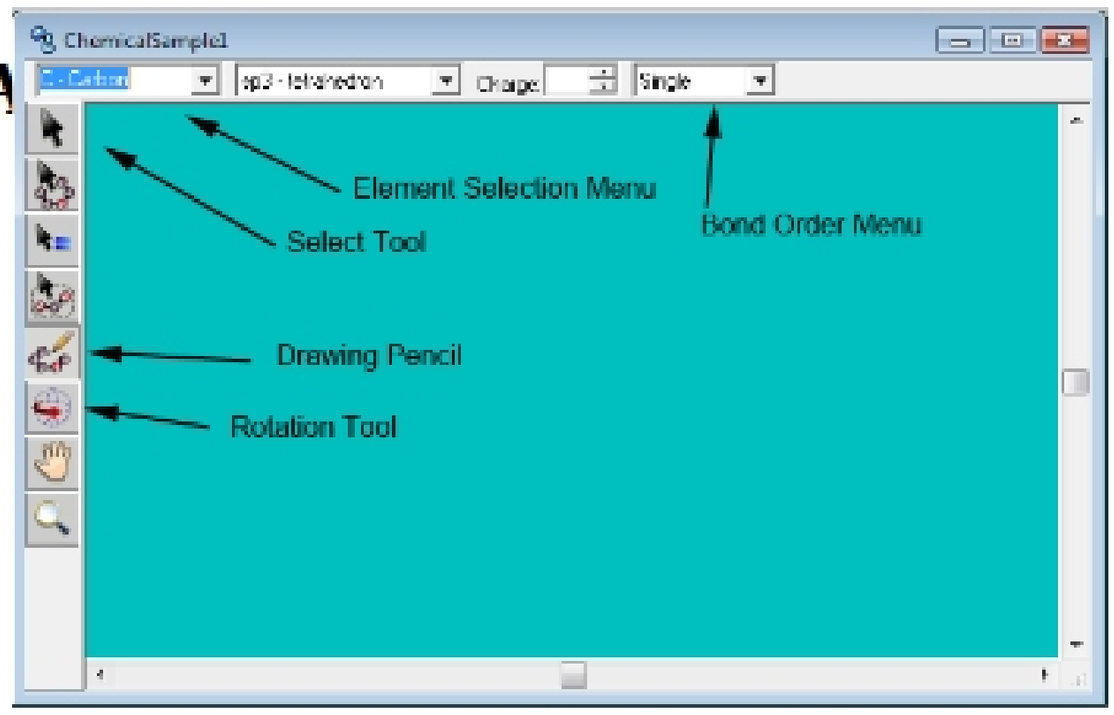
In this experiment you will learn how to:

- "build" molecules in the program
- analyze bond lengths
- analyze bond angles
- analyze torsion angles
- use these skills to perform an analysis of the structures of a series of small molecules.

Prelab Assignment

Before coming to lab, fill in the Lewis structures in Tables 1, 2A, 2B, and 4. Determine the formal charges and oxidation numbers requested in Table 4.

How to Use CA



1. Building Molecules

Run Workspace from either the CAChe or Scigress folders in All Programs. If a query comes up the first time, just say yes.

Choose **New** if a workspace window does not come up.

Use the **Drawing Pencil** to sketch out your molecule.

- To add the first atom, select the element and click in the middle of the workspace.
- To add addition atoms, select the element and then click-and-drag from the element you want it bonded to.
- To make a double or triple bond, either drag again between the two atoms, or use the Select tool to select the bond and change the drop-down menu to change it.
- Once complete, finalize the molecule using **Beautify/Comprehensive**, or Ctrl-B.

2. Performing Advanced Calculations (Experiments)

Save the molecule using a name of your choice.

Choose the **Experiment/New**.
Select the **Property** to be determined. Popular selections are “HOMO-5 to LUMO+4” and “electrostatic potential on electron density.”

Click Start and wait for the calculation to run its course. For small molecules this is usually less than 10 seconds.

Close the **Experiment** windows.

3. Making Measurements

Bond Length: select the two bonded atoms using the **Select** tool. Click on one atom, hold down shift, and click on the second atom. Then choose **Adjust/Atom Distance**, or press F2. The units used are Angstroms. 1 A = 10^{-10} m, or 10^{-8} cm.

Bond Angle: select three atoms- in order with the central atom second. Then choose **Adjust/Bond Angle**.

Torsion Angle: select four atoms- in order following the bonding linkages. Then choose **Adjust/Torsion Angle**.

Partial Charge: Build the molecule and save it. Run **Experiment/New/Property = current energy**. When the calculation is done, choose **View/Atom Attributes/Label/Partial Charge**. The numbers will be seen with the atoms. You’ll probably need to rotate the molecule to see them.