Chemistry 371 Lab Rybolt – Introduction to Molecular Modeling: Tutorial and Practice

Introduction

There are many different types of software that do molecular modeling which is a term that means using computer computation to determine structures and properties of molecules. The computations based on classical mechanics are often referred to as molecular mechanics with abbreviations such as MM1, MM2, MM3 etc. These are based on ball and spring models of interconnected atoms to make molecules. Parameters have been used to best represent the distance, angles, strengths, etc. of chemical bonds. The computations based on quantum mechanics have various degrees of approximations and those with more approximations are called semi-empirical methods that include specific applications of MOPAC. MOPAC with specific forms abbreviated as AM1, PM3, PM5, etc. can be used to find electronic distribution, orbital energies, orbital shapes, heats of formation, and structures of molecules. The specific software that we use at UTC is called Scigress (older name was CAChe for **C**omputer **A**ided **Che**mistry.) Scigress or CAChe has a user friendly interface that allows you to draw a molecule and then use mechanics or MOPAC to calculate structures and chemical properties. Additional information about molecular modeling may be found at http://vergil.chemistry.gatech.edu/courses/chem6485/index.html then select Intro to Molecular Mechanics (more detail) (from Dr. David Sherrill at Georgia Tech)

*Note the name of the software in use changed in 2008 to Scigress. **Scigress** is a new version of CAChe with slight modifications so as you read directions if a step doesn't work exactly as written then you will need to try a logical alternative or alternatives - please record any variations on these pages and share with instructor. Please consider any trial and error as part of the fun and challenge of the experiment. We may use the terms Scigress and CAChe interchangeably as it refers to same software. There is other software that does similar calculations ("Spartan" by company Wavefunction for example)

Any work you wish to save permanently must be saved on your OneNet account as the computer or your own floppy or CD. Files stored on the computer may be discarded several times during the year. When using Scigress it is necessary to save files on the computer. Open My Documents Folder on the desktop, create a new folder and give it your name. Save all files and documents only into your named folder.

Starting and stopping work in Chemistry Lab

*Login: use your UTCID and OneNet Password

To Start Scigress: double click Scigress Workspace on desktop

To Save Scigress file: choose File|Save as then locate My Documents folder then click on new folder and give it your name (JoeSmith) and then save all your Scigress files in your folder. ONLY SAVE into your own folder. You should save molecular structure files with appropriate molecular name.

If you are completely done with your folder and will no longer need any the items, you can place in RecycleBin (trash). All items will be removed from My Documents folder from time to time so nothing is permanent unless it is in your own OneNet Account.

To find fragment library go to →Program Files →Fujitsu→CAChe
Never save anything into fragment library!

*Logout before you leave: Ctrl + Alt + Delete brings up Logout page. Or choose Shut Down and then select Logout option. Do Not Turn Off Computer.

Learning to use Scigress

General Instructions
Whenever you draw a molecule it is good idea to use the full screen size to draw. After you have completed any new molecule, be sure to choose "select tool" from Tool Palette and click on background that will highlight entire molecule for further work. Then hold Ctrl and press f to center and size the molecule on the screen. After these actions, you should also rotate the molecule in a variety of ways to make sure that you have the correct desired three-dimensional structure. Save and refer to the Scigress User Interface for Windows Page as needed.

First - Scigress Tutorial
Follow the exercises labeled Exercises for Windows (there is a different Macintosh version) on the following pages. Complete the tutorial items I through IX. There are other more advanced computational techniques we are ignoring at this time. Do not continue until you have completed this tutorial. You need to know how to use this software for several experiments during semester.

Second- Applications
On separate sheets number questions and neatly record the answers for following questions on your own paper and be prepared to turn in this work for checking by your lab instructor. Instructor must be able to easily read and understand your report.

0) I have completed all the required portions of the Scigress Tutorial - yes or no

1) Draw a water molecule and Beautify. Use Toolbar options to view this molecules as Lines Only, Lines, Ball and Cylinder, and Space Filling. Draw a picture of each of these views and label.

2) Delete this water and draw a new water molecule that has one H very close to the O and one H very far away. H-O---------------------------------H Use "select tool" from tool palette and click on one H atom. Hold down shift key and then click on the oxygen atom. Then choose **Adjust - Define Geometry Label.** Repeat this prior procedure for other H and the O so that you now have a bond label on each H--O bond. Now click on background with "select tool" so entire

molecule is highlighted. Record each bond distance (the value is given in Angstroms). Choose **Beautify - Comprehensive**. Record the new bond distances for each bond.

3) Choose **Experiment - New** Save files - Yes. Name - Water. Within Experiment window choose chemical sample, optimize geometry, and MM3 from appropriate boxes. Click Start and observe calculation window. When done return to the molecule window and record the H--O bond distances.

4) Choose **Experiment - New** Save files - Yes. Name - Water. Within Experiment window choose chemical sample, optimize geometry, and PM5 from appropriate boxes. Click Start and observe calculation window. When done it will say "Tabulation Complete." Record the Heat of Formation calculated in kcal/mol. When done return to the molecule window and record the H-O bond distances.

5) Report the Heat of Formation of water calculated in kcal/mol that you found above and also report in units of kJ/mol. Locate the experimental value for the Heat of Formation for water in the gas phase $H_2O(g)$ in your textbook and record number and units. What is the percent error of the calculated value relative to the accepted experimental value?

6) Open a new window and draw a tribromomethanol molecule. CBr_3OH Repeat the above procedures for this molecule to get O-H bond length. Record the O-H bond distance after Beautify, MM3 mechanics calculation, and PM5 MOPAC calculation. Report these values. How do you account for these different O--H bond distances?

7) Go to the fragment library and pick out any medicinal molecule you wish. Paste this molecule on your screen as a ball and stick model with the atoms labeled by element type. Write the name of the molecule and do a Google internet search to find out what this molecule is used treat and one other interesting fact about it. Draw molecule by hand and report what it treats and the brief fact.

Scigress Reminders

a) To Start Scigress: double click Scigress Workspace on desktop

b) To Save Scigress file: choose File|Save as then locate My Documents folder then click on new folder and give it your name (JoeSmith) and then save all your Scigress files in your folder. ONLY SAVE into your own folder.

c) If you are completely done with your folder and will no longer need any the items, you can place in RecycleBin (trash). All items will be removed from My Documents folder from time to time so nothing is permanent unless it is in your own OneNet Account.

d) To find fragment library go to →Program Files →Fujitsu→CAChe

e) To define bond angle label:
Select Tool click on atom hold shift click on next atom and then third atom

Adjust|Bond Angle
Define Geometry Label
Unlock Geometry
Click OK

Or after atoms highlighted use toolbar shortcut Adjust|Define Geometry Label

f) To see valence electrons: View| Show Electrons

g) Always Ctrl f to center molecule after it is drawn. Always rotate the molecules to make sure you have the correct three-dimensional structure. You cannot be sure the molecule is what you want by just looking at flat geometry.

h) To optimize geometry:
Experiment|New
Then choose chemical sample, optimize geometry, PM5 or MM3 or other choice.

i) If doing anything to whole molecule such as running experiment or beautifying, make sure entire molecule is highlighted by using select tool and click on background.

j) To see atom distance:
Select Tool click on atom hold shift click on next atom
Adjust | Atom Distance
Define Geometry Label
Unlock Geometry
Click OK

Or after selecting atoms use toolbar shortcut Adjust|Define Geometry Label

k) When placing atom onscreen be sure to look at Element type box, Hybridization box, and Charge box. Look everytime or you will be entering incorrect values. Must be changed or updated after each atom is placed.

Hybridization and molecular structure
Read one page handout (at the end of this section) to review orbital geometry (also called electron pair geometry) and molecular geometry (shape based on atoms in molecule). Draw SF_6 and when S is placed use unconfigured in Hybridization box. The hybridization will be adjusted to the correct type based on total number of bonds and electron pairs when Beautify is done. Now beautify molecule by choosing Beautify|Comprehensive. For all items below be sure to choose to see valence electrons: View| Show Electrons. Seeing these electrons will help to understand geometry the molecule adapts. Use hybrid orbital designations in handout page: s sp sp^2 sp^3 sp^3d sp^3d^2. Scigress software may report in slightly different way for example d_zsp^3 to designate a specific d orbital orientation where we would just say sp^3d. Use the simpler notation (one on the information sheet that follows).

8) For SF_6 draw the final Lewis structure (show bonds by lines and valence pair electrons by dots) and report hybridization selected after Beautify.

Repeat above procedure for SF_5^- SF_5^+ SF_4^{2+}. Leave the center atom in unconfigured hybridization but the outer F or I should be selected to be sp^3. Put the extra molecular charge for ion on the central atom in each case. See reminder (k).

9) Draw Lewis structure (show bonds by lines and valence pair electrons by dots) and report hybridization for SF_5^-.

10) Draw Lewis structure (show bonds by lines and valence pair electrons by dots) and report hybridization for SF_5^+.

11) Draw Lewis structure (show bonds by lines and valence pair electrons by dots) and report hybridization for SF_4^{2+}.

12) Use the atom tool to draw a benzene ring structure C_6H_6. Draw carbon bonds as a set of alternating single and double bonds around the ring. Set each of the carbons to be sp^2 hybridization and the hydrogen atoms to be s hybridization. Beautify|Comprehensive and then place atom distance labels on one of the C–C bonds and one of the C=C bonds. Optimize geometry with MM3 and then PM5 and observe how the bond lengths change.

Report the <u>two bond lengths</u> after Beautify, MM3, and PM5 and explain why this change occurs and what it has to do with delocalized pi bonding in benzene.

13) Rotate benzene so it is flat on screen and you can see all 12 atoms. Draw the benzene molecule as ball and cylinder model. Toolbar has short cuts to all four different views.

14) Change to Space Filling and draw.

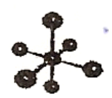
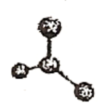
15) Change to Lines and draw

16) Change to Lines Only and draw.

REPRESENTATIVE VSEPR STRUCTURES

Orbital Geometry: describes the geometry of the orbitals, takes the nonbonding electron pairs into account because they must be in an orbital. The steric number and the hybridization will give the orbital geometry (electron-pair geometry). Therefore, there are only 5 possible orbital geometries: octahedral (sp^3d^2), trigonal bipyramidal (sp^3d), tetrahedral (sp^3), trigonal planar (sp^2) and linear (sp).

Molecular Geometry: uses the nonbonding electron pairs to describe the geometry of the molecule, use AXE notation.

Steric Number	Hybridization				
6	sp^3d^2	AX_6  **Octahedral** 90°	AX_5E  **Square pyramidal** equatorial: 90° axial/equatorial: <90°	AX_4E_2  **Square planar** 90°	
5	sp^3d	AX_5  **Trigonal bipyramidal** equatorial: 120° axial/equatorial: 90°	AX_4E  **See-saw** equatorial: <120° axial/equatorial:<90°	AX_3E_2  **T-Shaped** equatorial: <120° axial/equatorial:<90°	AX_2E_3  **Linear** 180°
4	sp^3	AX_4  **Tetrahedral** 109.5°	AX_3E  **Trigonal pyramidal** <109.5°	AX_2E_2  **Bent (angular)** <<109.5°	
3	sp^2	AX_3  **Trigonal planar** 120°	AX_2E  **Bent (angular)** <120°		
2	sp	AX_2  **Linear** 180°			

Steps for determining geometry: First, you must draw a correct Lewis Structure. Second, write the AXE notation. The molecular geometry will match up with the AXE notation. Third, determine the hybridization of the orbitals and the orbital geometry.