NOTE: For this laboratory, the student only needs to turn in the worksheet, the discussion of results, and the answers to the questions. No formal pre-lab or in-lab is necessary. However, the report must be typed and include the (typed) table of results.

Introduction to Molecular Modeling

Molecular modeling is a computational technique whereby the structure of a molecule is represented numerically and its behavior and properties are calculated using the equations of classical and quantum physics. These calculations are very complex, and in the past required the most powerful computers and significant amounts of computer time to carry out. Today, though, the typical PC is powerful enough to perform these calculations, and many software programs are available to carry out a variety of molecular modeling tasks. In these programs, the user draws a molecule of interest using a graphical interface, and he or she then uses the software to perform molecular mechanics calculations using classical physics, and to perform quantum mechanical calculations using either *ab initio* or semi-empirical methods. The results of these calculations are properties such as energy minima, heats of formation, interatomic distances, charge density maps, HOMO/LUMO maps, etc. for various conformations of the molecule of interest.

In this experiment, you will use Spartan – computer software which performs molecular modeling calculations – to construct molecular models and carry out calculations on four different compounds. Specifically, you will use molecular mechanics methods to calculate the strain energy (E_{strain}) for two conformations each of ethane, butane, cyclohexane, and *trans*-1,4-dimethylcyclohexane. In addition, you will use Spartan to determine certain other properties for the two conformations of the two cyclic molecules. You will then use this data to determine which conformation in each pair is the more energetically stable, and using what you have learned in class about conformational stabilities, you will provide a reasonable explanation for the results.

Using Student Spartan (Sims ACC Lab, Room 211)

To open Spartan, double-click on the **Spartan Student Version Icon** ( if available).

(Otherwise, open Spartan by clicking **Start → All Programs → Biology & Chemistry → Spartan ST**).

From the **Main Window**, select **New** from the **File Menu** (or click the **New** icon  in the toolbar) – this opens the *Build* window.

----Molecules are created in the build window using the tools on the right----

Select the **Tetrahedral Carbon** tool ().

Click in the build area to create a carbon (Methane).

----Atoms automatically have hydrogens (yellow) to complete the atom's valence----

Practice manipulating Methane.

To *move* a molecule, **Right-Click** and **Drag.**

To *rotate* a molecule, **Left-Click** and **Drag.**

You can *move* or *rotate* the molecule at any time while using Spartan.

When you are done practicing, select **Close** from the **File Menu** and Click **"No"** if the program asks if you want to save the file.

NOTE: Anytime you draw a molecule, look at it before you perform any calculations to make sure it is the molecule (and the conformation) you intended to draw. If it is not the correct molecule or conformation, your calculations will be misleading.

EXPERIMENT WORKSHEET

Data from Experiments	kJ/mol	kcal/mol
E_{strain} of Eclipsed Ethane	_____	_____
E_{strain} of Staggered Ethane	_____	_____
E_{strain} of Gauche Butane	_____	_____
E_{strain} of Anti Butane	_____	_____
E_{strain} of Chair Cyclohexane	_____	_____
E_{strain} of Boat Cyclohexane	_____	_____
E_{strain} of Diaxial *trans*-1,4-dimethylcyclohexane	_____	_____
E_{strain} of Diequatorial *trans*-1,4-dimethylcyclohexane	_____	_____

H1-H4 Distance in Chair Cyclohexane	_____
# of Eclipsing H-H interactions in Chair Cyclohexane	_____
H1-H4 Distance in Boat Cyclohexane	_____
# of Eclipsing H-H interactions in Boat Cyclohexane	_____
# of Gauche C-C interactions in Diaxial *trans*-1,4-dimethylcyclohexane	_____
# of Gauche C-C interactions in Diequatorial *trans*-1,4-dimethylcyclohexane	_____

Lab Report

This report must be typed (including a typed table of results). Convert the strain energies to kcal/mol and record these values in the worksheet and in your report. What does it mean for a conformation to be "more stable" than another conformation in terms of the strain energy? For each molecule, indicate the difference in strain energy between the two conformations. Compare the calculated energy differences for each conformation with the experimental values available in your lecture textbook (for 1,4-dimethylcyclohexane, the value available in your textbook is a calculated value). Discuss which conformation was more stable and why (be very detailed). For the boat and chair cyclohexanes, discuss how the interatomic distances and the number of H-H eclipsing interactions influence the stability of each conformation (again, be very detailed). For the 1,4-dimethylcyclohexanes, discuss in detail how the number of gauche C-C interactions influence the stability of each conformation. For each pair of conformations, did your modeling results confirm or contradict what you learned in class about conformational stabilities? How so? What can you conclude about the usefulness of applying molecular mechanics modeling to conformational analysis problems? *Include drawings of the appropriate conformations of all molecules to assist in your discussion.*