Experiment 8: Introduction to Physical and Computational Molecular Modeling

Reading for Week 1: Sections 8.1-8.5 in your textbook and this lab handout
Reading for Week 2: Sections 8.6-8.8 and 9.1-9.3 in your textbook (and this lab handout)
Materials: Bring your textbook and both pencils and a pen to lab each week

<u>Introduction To Computer Modeling (Gaussian/GaussView)</u>:

Molecular modeling is an invaluable tool for chemists to help them represent and visualize molecules (which are too small to be seen) and understand their behavior. Computational tools are available that are easy to use and give us the ability to build accurate chemical structures and calculate energies of these compounds, providing much insight into their properties and reactivity. This week, you will be introduced to a powerful computational program that is freely available to Colby students and faculty.

The computational program GaussView is a popular way to build virtual molecular models, submit these molecules for calculation, and analyze the results of those calculations. The calculations themselves are performed with a different software program called Gaussian. Instructions for using GaussView and Gaussian will be provided in the lab.

Once you become comfortable with the program, you can do many kinds of interesting modeling experiments. Furthermore, the structures and shapes of molecules, which may not be always obvious from our usual two-dimensional drawings, suddenly come to life on the computer screen. These models can be then viewed and probed in a variety of ways to gain a better understanding of the compounds that they represent.

Given below are a set of exercises that will not only help you learn the program, but also let you examine molecules in the context of what has been covered in class so far. Although you are only required to complete these exercises, you are invited – indeed encouraged – to branch out on your own and explore other compounds of your choice. Feel free to let your imagination run wild and make up all kinds of molecules even if they seem really crazy or silly. See how stable the compounds you made up are and how they look on the computer screen in three dimensions. Challenge your partner to see if she/he can come up with something even weirder than yours.

<u>Computational Experiments To be Completed in Week 1</u>

Part I: Diatomic molecules

- Build H_2, HF, HCl, HBr, HI, and Cl_2. Optimize the geometry at the default HF/3-21G level. Record the energy, bond length, charge distribution, and dipole moment of each molecule in your notebook.
- Using the equation given in your text (page 312), verify that the charge distribution corresponds to the dipole moment for any ONE of the hydrogen halides (HF, HCl, or HI). *Be sure to use the correct bond length.*

Part II: Structures of simple molecules

- Build and optimize water, ammonia, carbon dioxide, methane, and chloromethane. Record the energy, and all unique bond lengths, bond angles, and dipole moments for these molecules in your notebook.
- In your notebook, record the shapes of water, carbon dioxide, and methane.

Computational Experiments To be Completed in Week 2

Part III: Resonance structures

- Build and optimize the nitrate ion. Record its energy, bond lengths, bond angles, and dipole moment in your notebook.
- Build and optimize the acetate ion. Record its energy, bond lengths, bond angles, and dipole moment in your notebook.
- In your notebook, assign formal charges to all atoms in this ion and show your calculation.

Part IV: Reaction energies

Use the energies (heats of formation) that you calculated in Part II for methane, chlorine, hydrochloric acid, and chloromethane to calculate the the enthalpy change accompanying the reaction shown below. See the procedure on pg. 327-8 of your textbook if you need help.

$$CH_4 + Cl_2 \longrightarrow CH_3Cl + HCl$$

Introduction to Physical (Ball and Stick) Modeling:[1] You do not have to make a notebook entry or take notes/make observations for this section.

By using physical models, it is relatively easy to see both geometry and polarity, as well as to deduce Lewis structures. In this exercise you will assemble models for a sizable number of common chemical species and will use them to determine several features including geometry, polarity, isomerism and resonance.

The models you will use consist of wooden balls (atoms), pegs (single bonds), and springs (used for multiple bonds). The balls represent the atomic nuclei and inner core electrons. The pegs and springs represent valence shell bonding or nonbonding (lone pair) electron pairs. Most, but not all, of the non-hydrogen atoms in this exercise obey the octet rule. In their bonded structures, such atoms have four electron pairs around a central core and are represented in the model set as black balls with four holes. When these atoms participate in a multiple bond, more than one of their electron pairs (holes) are connected to the same atom. Springs are required for these bonds because of the rigid angles between the holes in these wooden atoms. A few of the structures will require "expanded octet" atoms. Atoms with an expanded octet can accommodate more than eight electrons. Atoms in the third and higher periods of the periodic table in the transition metal or representative groups (IIIA-VIIA) can have expanded octets. Initially we will assume that all heavy atoms obey the octet rule, and in our procedure we will *discover* the atoms that require "expanded octets". *Note: a more detailed set of instructions for using and analyzing ball and stick models will be provided when you arrive in the laboratory.*

Build the molecules contained in the worksheet that will be provided to you in lab, and fill in the requested information for each molecule. Your completed worksheet is due at the end of lab in week 2. *You are encouraged to use pencil to fill out your worksheet, and you may also use your textbook as a resource.*

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[1] Developed from "The Geometrical Structure of Molecules: An Experiment using Molecular Models" from *Chemistry 103 Laboratory Manual*, S.F. Sontum ed, Department of Chemistry and Biochemistry, Middlebury College, Middlebury, Vermont, 1988, pp 75 - 91.

What should be in your laboratory notebook?

1. The title for the experiment, name of your partner, and the date
2. The results from all computer calculations, and all related calculations from Parts I-IV

Laboratory report: No materials or report are due after week 1. At the end of the week 2 laboratory period, you will turn in your completed ball and stick model worksheet. After week 2, you will also write a report using the **Report Form** for Experiment 8.