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

Ongoing Learning Goals:
- To use a scientific notebook as a primary record of procedures, data, observations, and example calculations
- To present your formal results through a laboratory report along with proper citations

Additional Learning Goals for Experiment 8:
- To practice drawing Lewis structures and determining three dimensional structure, dipole moments, and formal charges for a variety of molecules and ions
- To execute simple computational modeling using Spartan to predict the structure and properties of molecules and ions

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

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 is provided as a separate document.*

Build the molecules contained in the worksheet that posted with this lab, and fill in the requested information for each WEEK ONE moleculse. *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.

Introduction To Computer Modeling:

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 Spartan is a popular way to build virtual molecular models, submit these molecules for calculation, and analyze the results of those calculations. A tutorial for Spartan is provided with the lab materials.

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.

Computational Experiments To be Completed in Week 1

Part I: 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.
- Save an image of the molecule as a jpg file.
- In your notebook, record the shapes of water, carbon dioxide, and methane.

Part II: Structure of DNA
- Use the biomolecule builder to construct a 20 nucleic acid sequence. Do not minimize the structure (it takes a long time).
- Save an image of the molecule as a jpg file.
- Can you see the major and minor groove of the DNA helix? Describe what you see.
- What atoms are present in DNA?

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-II
3. Images of any molecules that you built in Spartan.

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.