Accurate 3D Modeling of User Inputted Molecules Using a Hill Climbing Algorithm

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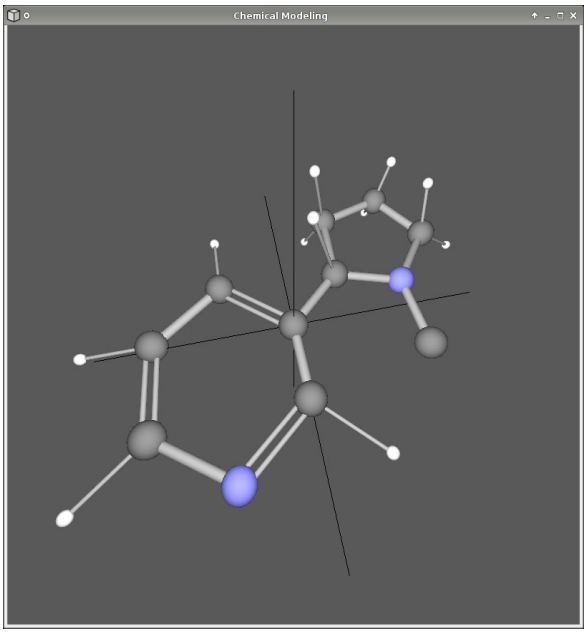
Abstract:

In order to better understand chemistry, chemists create 3 dimensional models of molecules. In a large introductory chemistry class, it is too costly to provide each student with a physical modeling set. Software available online can also be costly. The goal of my research project is to create a program that will allow users to generate 3D models of simple molecules through an intuitive and user friendly program. After the model is created, the program will then position the atoms in the molecule correctly by using a Nelder Mead algorithm. My project will help people, especially students, better understand the geometry of different molecules.

Background:

A lot of research has been done on modeling molecules and the techniques to do so now have become quite advanced. These programs have become increasingly more accurate over the years. However, the cost of these programs has also increased, and now very few people have access to them. For a beginning chemistry student there are not many options to play around with molecules and learn their different geometries.

One of the main features of my project will be the “Auto position atoms” function. This function will use a Nelder mead algorithm to minimize the energy of the model. The Nelder Mead algorithm was created by Nelder and Mead in 1965, and is uses the concept of a simplex in order to minimize a function in a many-dimensional space. A simplex is a polytope of N+1 vertices in N dimensions; therefore, it is a triangle in 2D space and a tetrahedron in 3D space. The algorithm begins with an original simplex. This simplex can not be too small, because it could lead to a local search. A simplex that is too large could a noticeably longer time.

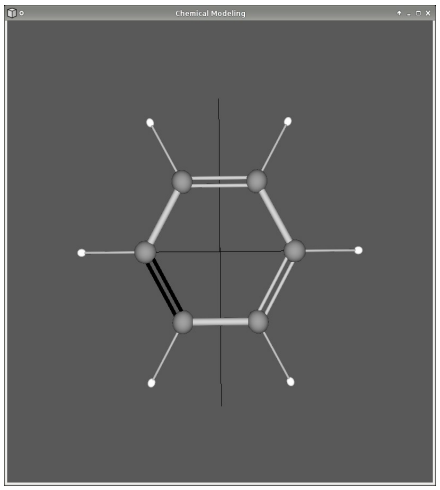


Nicotine ($C_{10}H_{14}N_2$)

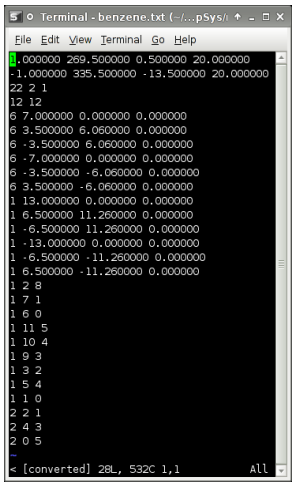
The energy function can be broken up into two parts. The first part is the distance of each atom to every other atom. The program will try to maximize this distance because real atoms do push away from each other. The second part is making the distances of bonded atoms a specific distance apart. This distance is specified in a data file and depends on what two atoms are connected and what type of bond exists between them. Since the Nelder Mead function tries to minimize the energy of the system, the minimum energy will occur when the atoms are as far apart from each other, except for bonded atoms which are the specified distance away from each other.

Methods:

Atoms are represented by spheres; bonds are represented by cylinders. Through inputs from the mouse and keyboard, users can create atoms and bonds, select and delete atoms and bonds, import and export models, draw single, double and triple bonds, choose which element they want to draw, and position the atoms where they want. The Nelder Mead function is used to “Auto position atoms.”



Benzene (C_6H_6)



Exported Benzene file

Results:

The purpose of my project is to create a free program that will allow users to easily and intuitively create models of molecules. Then, after a user finished creating the molecule, the program will correctly position the atoms. My project currently allows users to create molecules. A user can also rotate the model and zoom it in and out. These functions help users get a better picture of the molecule. I have also finished programming the Nelder Mead algorithm. The focus for fourth quarter will be programming the energy function and the original simplex, and then thoroughly testing the “Auto position atoms” function.