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 3D models of molecules. In a large introductory chemistry class, physical models are not viable because the supplies needed to give each student the opportunity to create even simple molecules are too costly. Also, software available online can also be costly. The goal of my research project is to create a program that will allow users to generate accurate 3D models of simple molecules (i.e. not macromolecules). Therefore, my project could help students in introductory chemistry courses better understand the geometry of different molecules.

Background:

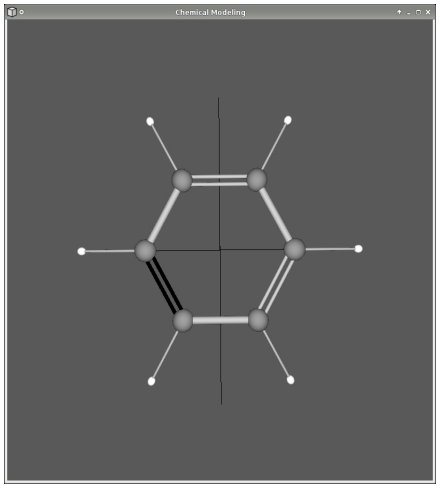
A lot of research has been done on modeling molecules and the techniques to do so now have become quite advanced. Pharmaceutical companies have invested thousands of dollars in programs to predict orientations of new complex molecules. Large databases have been created, storing the orientations of thousands of molecules. Chemists have modeled everything from RNA to inorganic crystals. 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. buying physical modeling sets for everyone in a introductory chemistry course is costly. Also, software on the Internet can also be costly, sometimes a couple hundred dollars. Therefore, even today, a free program to model simple molecules would be helpful.

Methods:

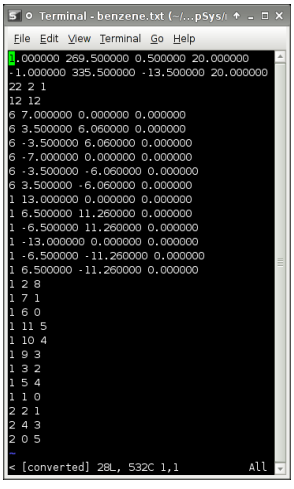
Atoms are represented by spheres; bonds are represented by cylinders. Through inputs from the mouse and keyboard, users can create atoms and bonds, select and delete atoms and bonds, import and export models, draw single, double and triple bonds, choose which element they want to draw, and position the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

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 the 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. However, I still need to work on the algorithm to correctly position the atoms. This will be the focus of the third quarter.



Benzene C_6H_6



Exported Benzene file