

# Computer Systems Project Proposal: Accurate 3D-Modeling of User Inputted Molecules

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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. The goal of my research project is to create a program that would generate accurate 3D models of simple molecules, avoiding the cost problem with physical models. Therefore, since it is hard to find a modeling program that is free, my project could help students in introductory chemistry courses better understand the different shapes of molecules.

## **1 Introduction**

### **1.1 Scope of Study**

The first step to my project was creating the graphics for my models. The graphics for my project are a much simplified version of real molecules: spheres represent atoms and cylinders represent bonds. Nevertheless, the results are sufficient.

The second step of my project is creating the algorithm that will correctly orient the atoms in the molecule. Since there are many variables accounting for the actual orientation of the atoms and because I only have a limited amount of time, I will need to limit the number of accounted variables. With

my set number of accounted variables, I will use an A.I. algorithm (hill-climbing) to correctly orient the atoms in the molecule. The first variable that I will account for will be the polarity of the bond. Once I get that working, I will continue to add more variables, creating a better model.

## **1.2 Expected results**

My project tries to avoid the problems with creating physical models of molecules by creating them on the computer.

This project combined many of my interests: 3D graphics, A.I. and chemistry. This project will help me integrate my interests, even though they all do not directly link to computer science.

## **1.3 Type of research**

My project is pure applied research; it is motivated by use. The goal of my program is to provide introductory chemistry students the ability to easily create accurate models of simple molecules.

# **2 Background and review of current literature and research**

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. Therefore, even today, a free program to model simple molecules would be helpful.

# **3 Procedures and Methodology**

Now that I have most of the graphics done for my project, I will now be able to start working on my algorithm to correctly orient the atoms in the

molecule. I will first start by only taking one variable into account: the polarity of the bond. Once I get that working, I will then add another. Once that one is working, I will start on another. Through this process, my program will start to produce accurate representations of different molecules.

The graphics part of my project will construct the visuals portraying the output of my algorithm for orienting the atoms.

In order to see if my program is constructing accurate models, I will compare my models with the actual/accepted models. By doing this, I will also be able to do error analyses. In order to thoroughly test my program, I will test many different molecules and compare my results with the actual orientations.

Dynamic testing will not work for my project because an atom can not bond with any random atom. Therefore, I will mostly use specific structural and functional testing and path and branch testing.

## 4 Expected Results

My project will allow users to create accurate models of simple molecules with just a few clicks. After the creation of the molecule, users will be able to rotate it and zoom it in and out in order to get a better picture of the molecule.