

# Accurate 3D Modeling of 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.

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

## Methods:

Atoms are represented by spheres; bonds are represented by cylinders. Mouse inputs are used to control rotations and zooming.

## Results:

Models can now be created by editing the source code. The pictures below are two molecules that I have created. These models are lighted and colored, and are rotatable and zoomable.

