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7 October 2016
MATH 198

Pre-Proposal

1 General concept

Cyclohexane is a particularly interesting molecule in organic chemistry. Its ringed structure is unique in that it is actually as stable as a linear molecule, which cannot be said for most other ringed structures.

Figure 1: The planar structure of cyclohexane

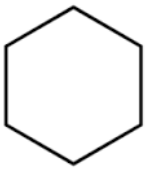
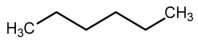


Figure 2: Linear hexane

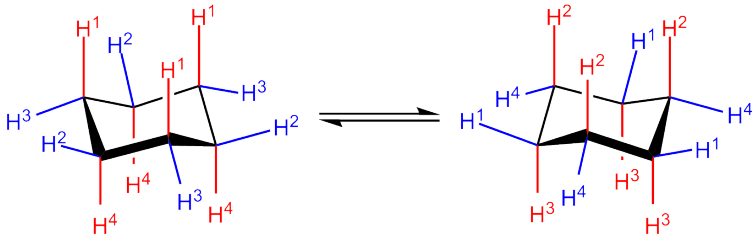


However, cyclohexane does not exist as a perfect hexagon. Rather, it is a complex three-dimensional molecule that is better represented by a figure called the chair conformation. Like all

Figure 3: The chair conformation of cyclohexane

other carbon-carbon single bonds, the carbons of cyclohexane undergo rapid rotation at room temperature. However, in this cyclic conformation, the rotation of one carbon induces a rotation in neighboring carbons, leading to very unique interconversions.

Figure 4: The interconversion of cyclohexane in the chair conformation. Axial hydrogens are in red and equatorial hydrogens are in blue



Furthermore, each hydrogen on each carbon in cyclohexane undergoes its own conversion during the overall chair conformation interconversion. The hydrogens, or any substituent groups off one of the carbons in cyclohexane, can be in an equatorial or axial position. In the above figure, the axial hydrogens are in red and the equatorial hydrogens are in blue. During the chair interconversion, the axial hydrogens actually become equatorial, and the equatorial hydrogens become axial. Thus, the chair interconversion is a complicated transition.

2 Implementation in VPython

The carbon atoms and hydrogen atoms in cyclohexane are most easily visualized as balls and the carbon-carbon bonds and carbon-hydrogen bonds are best represtented as sticks. A working and accurate model of cyclohexane can be created using spheres and cylinders in VPython. Furthermore, to analyze the movement of hydrogens on each carbon in cyclohexane, this model of chair can be animated to show the transition of one chair conformation to the other. Using VPython, a more accurate model of the chair interconversion can be described and help visualize the complicated interconversion of the carbon and hydrogen atoms. This process will likely combine principles of past projects involving atomic structures as well as analysis of many "blobby man" projects, which involve coordinated and synchronized movements of different objects together (i.e. the arm and hand of the blobby man must move together while he is swimming.)

3 Goals

For the final project, I hope to accomplish (at the minimum)

- A three-dimensional depiction of the interconversion of the forms of the chair conformation of cyclohexane
- The animation of this interconversion

If time permits and if the project is feasible, I also hope to

- A three-dimensional depiction of both the axial and equatorial hydrogens on each carbon in cyclohexane
- The animation of the interconversion of these hydrogens from equatorial to axial during the chair interconverison

Lastly, for a potential challenge, if the previous goals are accomplished, I hope to

- A three-dimesnional depiction of different kinds of substituents on each carbon besides hydrogen (*e.g.* methyl groups, ethyl groups, various functional groups with atoms besides carbon and hydrogen)
- The animation of the interconversion of cyclohexane with the movement of these larger substituents