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MATH 198

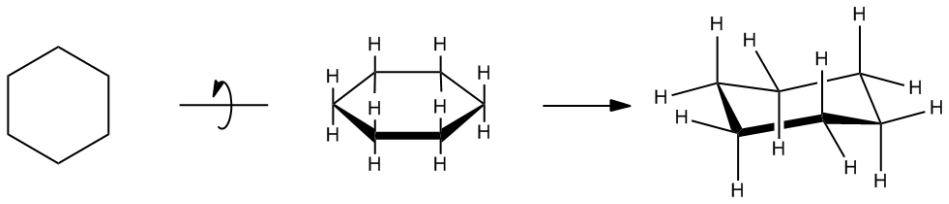
Animating the Interconversion of Cyclohexane

Contents

1 Abstract

My project consists of an animation in VPython of the movement of cyclohexane (chair conformation interconversion) between two of its three-dimensional shapes. This animation is summarized in the figure below. [1] The animation will unite concepts of defining scenes and frames and moving various shapes in concert. I integrated the concepts of past blobby projects to apply the movement of concerted shapes in a more complicated context.

Figure 1: A summary of the visualization of cyclohexane



[1] All images are from `www.masterorganicchemistry.com` [2].

2 Background

Cyclohexane is a particularly interesting molecule in organic chemistry. Its ringed structure is unique in that it is actually as *stable* as its linear counterpart, hexane, which cannot be said for most other ringed structures. There are multiple factors in considering stability of chemical molecules [1].

Figure 2: The planar structure of cyclohexane

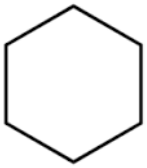
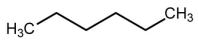


Figure 3: Linear hexane

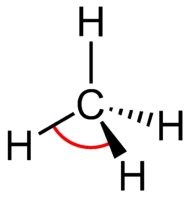


2.1 Bond angles

Firstly, in considering chemical stability, there is the issue of bond angles, particularly with ringed structures. Ringed structures are a common occurence in chemistry. However, atoms and bonds twisting cause strain on the molecule by disrupting the bonds between atoms, so the molecule will adjust to a conformation that minimizes that strain. The ideal bond angle is 109.5 degrees, as illustrated by the methane molecule. This angle minimizes strain between the hydrogens and the central carbon atom.

The table below describes several ringed structures in chemistry, as well as their bond angles. Molecules like cyclopropane and cyclobutane have bond angles that deviate so greatly from the ideal that they are highly unstable in nature. These molecules are both incredibly reactive. Cyclopentane is closer to the ideal bond angle of 109.5, which is why it is stable. Cyclohexane, however, is incredibly unique in that it exactly matches the ideal bond angle. This ideal

Figure 4: Methane, or four hydrogen atoms on a central carbon atom



bond angle gives cyclohexane many unique properties, as a result of its enhanced stability.

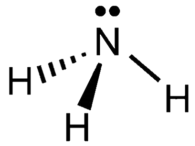
Structure	Name	Bond angle (in degrees)
	Cyclopropane	60
	Cyclobutane	90
	Cyclopentane	108
	Cyclohexane	109.5

2.2 Electron repulsion

Another factor in determining conformation is electron repulsion between atoms. It is known that molecules will conform to certain shapes in order to minimize the electron repulsion between atoms. By minimizing these repulsions, the molecule also minimizes its potential energy.

Ammonia also has four groups around the central atom, but one of these groups is a lone pair. This lone pair repels the electrons in the hydrogen atoms, leading to bond angles of approximately 107 degrees. Although this deviates from the desired 109.5 degrees, ammonia is still stable because electron repulsion is minimized. Thus, electron repulsion can cause a deviation from the ideal bond angle that still allows for stability.

Figure 5: Ammonia, a nitrogen atom with a lone pair of electrons



2.3 Bond rotation and chair interconversion

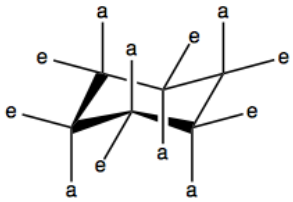
Cyclohexane is not a perfectly planar hexagon. In order to adapt the ideal 109.5 degree bond angle, the carbon atoms in cyclohexane are twisted out of the plane in a conformation known as *chair conformation*.

Figure 6: The chair conformation of cyclohexane

Like all other carbon-carbon single bonds, the bonds of carbons of cyclohexane undergo rapid movement at room temperature. However, in this cyclic conformation, the movement of one carbon induces a movement in the carbon atoms connected to it. Thus, this normal molecular movement is slightly more involved in cyclohexane and in all cyclic molecules.

Furthermore, each hydrogen on each carbon in cyclohexane experiences its own movements during the overall chair conformation interconversion. The hydrogens can be in two distinct positions, *equatorial* or *axial*.

Figure 7: Equatorial groups are labeled e. *Axial groups are labeled* a.

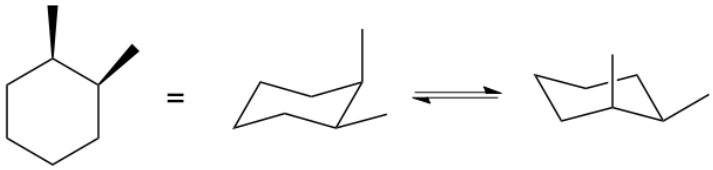


These hydrogens are all exactly identical; the terms equatorial

and axial are simply used to define their location in space relative to the carbon atom to which they are connected. If the hydrogen is directed along the y axis relative to the carbon, the hydrogen is considered axial. Otherwise, the hydrogen is equatorial. During the chair interconversion, the axial hydrogens actually become equatorial, and the equatorial hydrogens become axial.

This concept of atoms attached to the carbon atom in cyclohexane going from equatorial to axial during the chair conformation interconversion applies also to groups other than hydrogen atoms. In the figure, a chemical group attached to the carbons converts from equatorial to axial, as seen in the figure below.

Figure 8: Interconversion of cyclohexane



3 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 was 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 combines principles of past projects involving atomic structures as well as analysis of many "blobby man" projects, which involve coordinated and synchronized movements of differen objects together (i.e. the arm and hand of the blobby man must move together while he is swimming.)

4 Final Project

For the final project, I accomplished a three dimensional depiction of the interconversion of the forms of the chair conformation of cyclohexane and the animation of this interconversion.

5 Appendix

References

[1] Marc Loudon, *Organic Chemistry*. Purdue University, Roberts and Company Publishers, Colorado.

[2] Master Organic Chemistry
`www.masterorganicchemistry.com`