Hexane Conformers

Cañada College Virtual Lab

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Overview

The chair and boat conformers of cyclohexane will be explored using the visualization tool Avogadro. Avogadro is a program which allows you to create and view three-dimensional molecular structures. It also contains an algorithm which simulates how bonding and through space interactions contribute to the relative energy of different conformers. Using this program you can measure the distance between atoms to predict which conformers would be higher in energy than others. You will also be able to see how higher energy conformations would reorganize into a lower energy structures.

Using Avogadro

To launch Avogadro, double click on the application link on the desktop or select Avogadro from the start menu. When you open Avogadro you will see a central view window with a black background and nine tool icons to the left of the window. Selecting the different tools will give you different options and change how Avogadro interprets mouse clicks and drags in the editing window.

The nine tools are: Draw, Navigate, Bond Centric, Manipulate, Select/Rotate, AutoRotate, AutoOptimize, Measure, and Align. For this lab you will only be using the four tools: Draw, Manipulate, Optimize, and Measure.

Draw Tool: The draw tool allows you to create and change molecular structures. Click on the draw tool to make it active. The draw tool allows you to choose both bond order and atom type with the two pop-up menus. When the draw tool is active, clicking in the editing window will create a new atom of the type selected in the atom type pop-up. Clicking on an existing atom will change the atom type to the type of atom selected in the atom type pop-up. Clicking on an atom, holding down the mouse, and dragging to another atom will create or change a bond between the two. The new bond will be of the type selected in the bond type pop-up. Clicking on existing atom, holding down the mouse button and dragging to an empty space in the window will create a new atom bonded to the original atom. If the "adjust hydrogens" tool is active the number of hydrogens around most atoms will be set automatically based on atom and bond type.

Test the tool. Make sure the atom tool is set to carbon and the bond tool is set to a single bond. Make sure the adjust hydrogen tool is activated. Click in one space to create a methane molecule. Click on the carbon, hold down the mouse, and drag to another part of the window to create an ethane molecule. Click on the new carbon and drag to another place in the window to add a carbon to make propane.

Manipulate Tool: The manipulate tool is the fourth tool in the menu. This tool let's you move atoms in space. When the manipulate tool is selected you can click and drag an atom to move it up, down, right or left. When you hold down the shift key and then click and drag on an atom you an move it towards you (out of the screen) or away from you (into the screen).

Test the tool. Click on a carbon atom in your propane structure and move it to another location in the window.

Optimize Tool: The optimize tool allows you to activate a molecular mechanics force field. This is a powerful computational simulation that will make the atoms of your structure behave as if they were real atoms, pulling together along bonding interactions and pushing against each other to mimic steric effects. The optimize tool works by making small changes in the position of the atoms of your structure and calculating the energy before and after the change. If the change lowers the energy, the molecule keeps the change and looks for another one, if the new energy is higher the molecule reverts back to it's original shape.

You have different choices in how you optimize your molecule. The optimize tool allows you to select from three force fields: Ghemical, MM94 (molecular mechanics force field 1994), and UFF. Each is a different way of calculating energy of the structure. You can also choose which algorithm you want Avogadro to use to move the molecule. For today's lab use only the "steepest descent" algorithm. Keep "fixed atoms are moveable" and "ignored atoms are moveable" option turned on. There is also an option to set how many changes the force field makes before the picture is updated, leave the steps per update on "4" for today's experiment.

When the simulation is turned off, you can click and drag on the viewing window to rotate our molecule. When the simulation is active, you can click and drag to pickup and move atoms (this is useful to make small adjustments to a molecule if it "gets stuck' in a strange conformation).

Test the tool. Choose the MMFF94 option for force field, 4 steps per update, and steepest decent algorithm. Make sure the two check boxes are checked. Before you start the simulation, click and drag in the window to rotate the atom so you can more easily see how the simulation will change the two carbon carbon bonds. Click start. Watch how the molecule reorganizes itself into the more familiar shape of propane. Click and drag a carbon atom. When you release the atom watch how the simulation snaps it back into an optimal position. When the molecule appears to stop changing it's reached a stable conformation. Click the stop button to stop the simulation.

Measure Tool: The measure tool allows you to easily measure the distance between atoms and determine bond or dihedral angles. When the measure tool is active you can click on two atoms and their distance (in angstroms) will be displayed in the lower left corner of the screen. If you click on a third atom, both the distance from the first to second and second to third atoms will appear at the bottom of the window. The program will also display the angle between the first, second and third atom. Clicking on a fourth atom will display three distances two bond angles, and also the dihedral angle between the first two atoms and the last two. Clicking off into space will deselect all atoms and reset the measure tool to allow you to start a new measurement.

Try the tool. Click on a hydrogen and a carbon connected to it. What is the C-H bond distance in propane? Reset the measure tool. Click on a terminal carbon and then on the central carbon in your propane structure. What is the C-C bond distance in propane? Click on the third carbon without resetting the measure tool. What is the C-C-C bond angle? (Save these numbers, you will be asked for them in step 1 of the experiment)

Experiment

Step 1) Launch Avogadro and construct molecule #1: propane. Optimize propane to make sure you have a reasonable structure for the molecule. You should have already done this if you followed the "test the tool" directions in the using Avogadro section above. Measure and record the following:

Measure and record the following for propane:
a) measure the C-H bond length ____________
b) measure the C-C bond length ____________
c) measure the C-C-C bond angle ____________

Step 2) Look at molecule #2: the chair conformation of cyclohexane. The chair conformation of cyclohexane has already been constructed for you. Read the molecule file into Avogadro by selecting Open from the file menu and finding the Hexane Modeling folder (it will be either on the desktop of your computer or in the canchemistry user folder). Browse inside this folder and double click on the file named "hex-chair.cml." Activate the optimization tool but do not start the simulation. Rotate the molecule. Make sure what you are seeing is a cyclohexane chair conformation. Start the simulation, the molecule should change only slightly. If the molecule is not changing significantly stop the simulation and rotate the molecule so you can easily see three carbon atoms. Activate the measure tool.

Measure and record the following for cyclohexane chair conformation:
a) measure the C-H bond length ____________
b) measure the C-C bond length ____________
c) measure the C-C-C bond angle ____________

Step 3) Compare your measurements for molecule #1 and molecule #2. Are these measurements similar? What do you conclude about cyclohexane's chair conformation?

Step 4) While still in the optimize tool, rotate molecule #2 and look along two bonds (like a Newman projection), are the hydrogens staggered? Rotate and look along another two bonds, are the hydrogens staggered? What can you say about the relationship between adjacent hydrogens in cyclohexane and how does this compare to their arrangement in propane?

Step 5) Hydrogen atoms that are closer than 2.40 A in space will interact, creating steric strain. What is the distance between axial hydrogens? What is the distance between adjacent equatorial hydrogens? Are any of the hydrogen atoms in molecule #2 close enough to create this strain?

Measure and record the following distances:

a) distance between axial hydrogens ____________
b) distance between adjacent equatorial hydrogens ____________
c) distance between adjacent equatorial & axial hdyrogens ____________

Step 6) Look at molecule #3: the boat conformation of cyclohexane. The boat conformation of cyclohexane has already been constructed for you. Read the molecule file into Avogadro by selecting Open from the file menu and finding the Hexane Modeling folder (it will be either on the desktop of your computer or in the canchemistry user folder). Browse inside this folder and double click on the file named "hex-boat.cml." Activate the optimization tool but do not start the simulation. Rotate the molecule. Make sure what you are seeing is a cyclohexane boat conformation. Do not optimize this structure. Activate the measure tool.

Measure and record the following for the cyclohexane boat conformation:

a) measure the C-H bond length ____________

b) measure the C-C bond length ____________

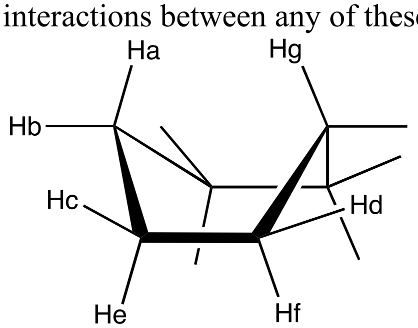
c) measure the C-C-C bond angle at peaks ____________

d) measure the C-C-C bond angle at lower corners ____________

How do these values compare to those of propane?

Step 7) Activate the optimize tool but do not start the simulation. Rotate molecule #3 so you can look along the two parallel bonds. Are the hydrogens staggered or eclipsing? How does this compare with propane?

Step 8) Measure the distance between hydrogens in molecule #3. Are there steric interactions between any of these hydrogens (if so, which ones)?



H_a-H_g distance ____________

H_b-H_c distance ____________

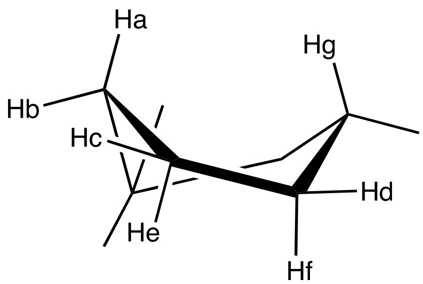
H_c-H_d distance ____________

H_b-H_e distance ____________

H_e-H_f distance ____________

 last updated 09.26.2009 by N. DeMello

Step 9) Turn on the simulation and minimize structure #3. The simulation should reshape the conformer into a twist boat. When the simulation stops making changes to the molecule stop the simulation. Rotate the molecule, is it a twist boat? Repeat your measurements. What steric interactions remain?



H_a-H_g distance ______________

H_b-H_c distance ______________

H_c-H_d distance ______________

H_b-H_e distance ______________

H_e-H_f distance ______________

Conclusions: What are your conclusions about chair, boat, and twist boat conformations? Which conformation would you say is the most stable and which is the least? Explain why you made these choices.

last updated 09.26.2009 by N. DeMello