Chem 232

Conformational Analysis & Representation of Cyclohexanes

Drawing the Perfect Chair Cyclohexane

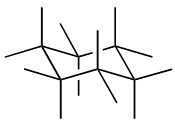
Drawing a perfect chair cyclohexane takes a little practice, but the rules for doing it are simple. Follow them, and you will soon be an expert. What makes a professional-looking chair?

Note the following features in the examples below:

- All bonds are drawn at one of four angles -- the ring defines three of the angles, and the other angle is 90o (straight up and down).
- Each edge of the chair is parallel to the one opposite it.
- Equatorial bonds are perfectly parallel to the ring bonds that are one bond away.
- Axial bonds alternate up and down around the ring. If the perspective is just right, the horizontal spacing between the axial bonds will be even.
- Where two bonds cross, the one in back is broken to emphasize perspective.
- Bond lengths are equal.
- The bottom half of the ring is closer to you. Ring bonds may be wedged for emphasis as shown at right, but this is not at all necessary.
- The chair may be drawn as either of two mirror image forms. Most of the time, you can draw whichever one is easier.
- A line drawn between the top two carbons is horizontal and parallel to a line drawn through the bottom two carbons. (A chair can actually be drawn at any angle, but horizontal is easiest.)

If you draw things this way, you will not need wedges or dashes for the bonds to axial and equatorial substituents -- the wedges and dashes will only make your diagram confusing. A how-to guide to drawing chair cyclohexanes is provided on the back of this page.

Perfect Chair



Mirror Image Also Perfect

With Perspective Emphasized

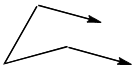
Mirror Image

Here's a step-by-step guide to drawing a cyclohexane chair:

Step 1

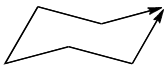
Start with a tilted "V." The angles of the lines are about 15° and 60° with respect to horizontal.

Step 2



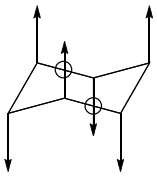
Draw two parallel, downward slanting lines at an angle of about minus 15°.

Step 3



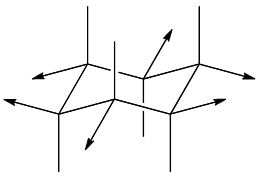
Finish with a pair of lines parallel to the first two.

Step 4



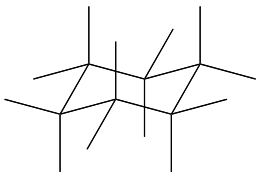
Add the axial bonds, introducing breaks where bonds cross (circled). You will need to erase part of one ring bond. With practice, you will learn to leave a gap in this bond as you draw it.

Step 5



Make the equatorial bonds point away from the ring. Of your four allowed angles, there will be only one left to choose at each atom.

Done!



Drawing Ring Flip Isomers

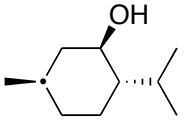
Drawing the two ring flip isomers of a substituted cyclohexane is easy if you do it systematically. The most important things to realize are:

a. Every substituted cyclohexane compound has exactly two ring-flip conformers. Upon ring flip, all axial groups become equatorial, and all equatorial groups become axial. Don't be afraid to put groups into the axial position if that's where they have to go. Don't wish them into being equatorial!

b. There is no direct correlation between up/down in the skeletal structure and axial/equatorial in the chair structure. A given substituent will be axial in one ring flip isomer and equatorial in the other, irrespective of whether it is up or down in the skeletal structure. *The correct up/down relationships in the skeletal structure must be preserved in drawing the two conformers.*

Here is an example of how to draw the ring-flip isomers of menthol, a trisubstituted cyclohexane.

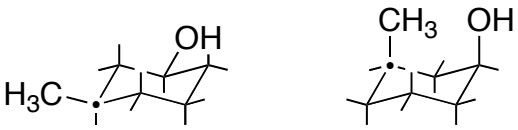
1. Pick any atom on the ring that has a substituent and mark it (I picked the one that has the methyl substituent). This will be your reference atom.



2. Draw two identical chairs. The first few times you do this, draw bond stubs to mark the positions of all 12 substituents to help orient yourself. Pick any carbon in the first chair and mark it. Go to the corresponding atom in the second chair, move one carbon in either direction around the ring, and and mark that atom (I moved clockwise).

3. Add the first substituent to the marked carbon on both chairs. In the example, it is an up methyl. On the chairs, the up substituent at a given atom is always the one drawn higher on the page. Up is equatorial on the left chair and axial on the right chair.

4. Move around the ring to the position of the next substituent. Here, moving two carbons clockwise brings us to a carbon with an up hydroxyl. Moving the same number of atoms in the same direction on your chairs, find the corresponding positions and add the substituent to each chair. Up is again equatorial on the left and axial on the right.



5. Move one atom further around the ring to the final substituent, a down isopropyl group, and preferably, erase the unused bond stubs. In this case, down is equatorial on the left and axial on the right.