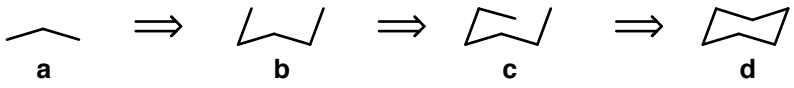
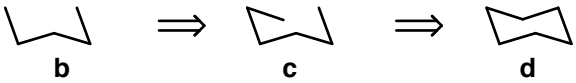
Chair Cyclohexane Tutorial — Solutions

1. Learn to draw a correct chair.

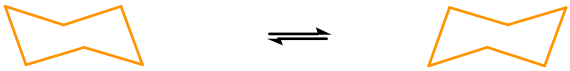
a. Start by drawing a 3C chain with a wider than usual bond angle.
b. Add parallel bonds to each side slanted approximately 20°.
c. Add a bond on the top left that is parallel to the bond on the bottom right.
d. Add the final bond on the top right that is parallel to the bond on the bottom left.



The other chair conformation can be drawn by tilting the bonds in step "b" to 20° in the other direction.



Now you try drawing both ring flip conformations:



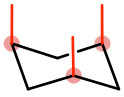
2. Be able to identify "up" carbons and "down" carbons.

If the two bonds of the ring attached to a carbon are pointing upward, the carbon is an "up" carbon.
If the two bonds of the ring attached to a carbon are pointing downward, the carbon is a "down" carbon.

You Try: In each chair below, put a circle around every "up" carbon and a triangle around every "down" carbon

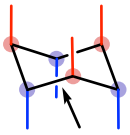
3. Be able to draw in axial and equatorial substitutents on a chair

Start with axials:
On every "up" carbon, the axial is pointed straight up.
On every "down" carbon, the axial is pointed straight down.



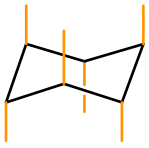
Draw the "up" axials on the "up" carbons.

Draw the "down" axials on the "down" carbons.



notice the "break" in the bond to indicate that it is behind the front bond of the ring.

You Try: Draw in the axial substitutents on the other chair conformation.

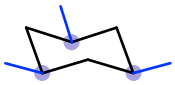


3. Be able to draw in axial and equatorial substitutents on a chair

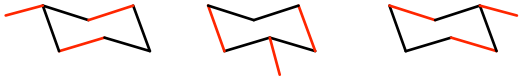
Now for the equatorials.
On every "up" carbon, the equatorial is pointed down and to the side.
On every "down" carbon, the equatorial is pointed up and to the side.

Draw the "down" equatorials on the "up" carbons.

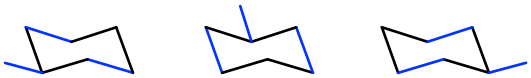
Draw the "up" equatorials on the "down" carbons.



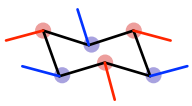
Ensure each equatorial is parallel with a bond of the ring!

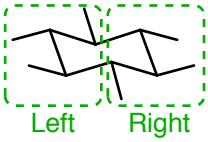


Again, ensure each equatorial is parallel with a bond of the ring!



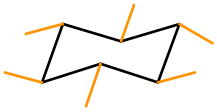
Drawing in all six equatorial bonds together:





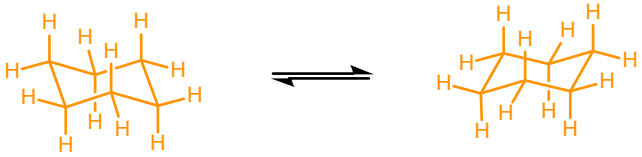
Notice: the three equatorial bonds on the left side point to the left, and the three equatorial bonds on the right side point to the right.

You Try: Draw in the equatorial substitutents on the other chair conformation.

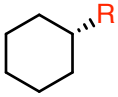


4. Be able to put it all together.

You Try: In space below, draw both ring flip chair conformations. Then draw all six axial bonds and six equatorial bonds on each. Finally draw in the twelve hydrogen on each axial and equatorial bond.

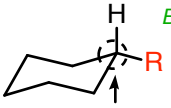


5. Be able to draw both chair conformations of mono-substituted cyclohexanes.

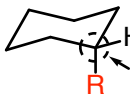


If the group is "back," translate it as a "down" group on the ring. It may end up axial or equatorial depending on which carbon of the chair you place it on.

Both are perfectly vaild chair conformations.



On this carbon, the "down" group is equatorial.

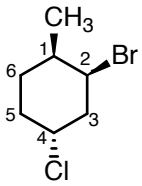


On this carbon, the "down" group is axial.

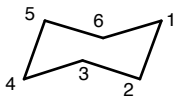
You Try: Draw chair conformations for the molecule below putting the ethyl group at the indicated positions on each chair.

6. Be able to draw a chair conformation containing two or more substituents.

a. Start by numbering your ring. This is just for bookkeeping, but you can use the IUPAC system if you wish.

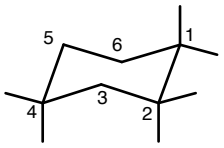


b. Number your chair in the same direction (clockwise or counterclockwise) as the numbering in your "flat" ring.

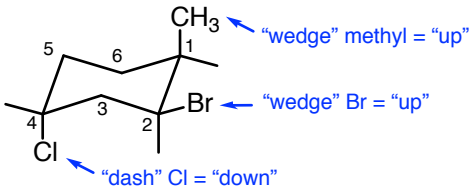


Note: You can make any carbon on the chair #1. Regardless of which one you pick, you will still get a valid chair.

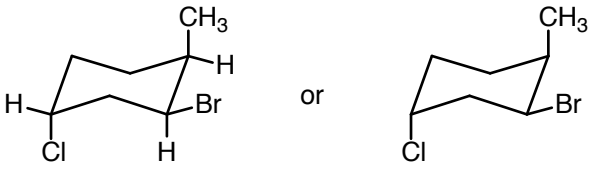
c. Draw in substituent bonds on all numbered carbons containg a substituent.



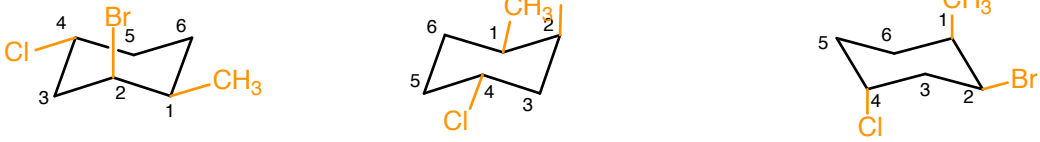
d. If the substituent is a "wedge," draw it in as an "up" substituent on the chair. If it is a "dash," draw it as a "down" substituent.



e. Finish the chair by drawing in H's on the remaining substituent bonds. Alternatively, erase these bonds to leave the H's implied.

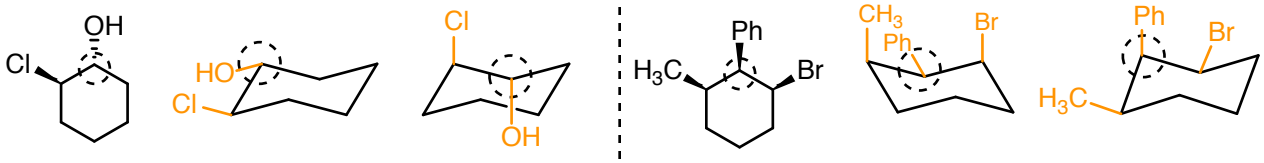


You Try: Draw valid chair structures for the molecule above using the alternative numbering positions on the chairs below.



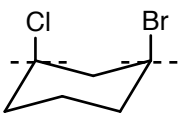
Note how I maintained a clockwise numbering in all cases because that is how I numbered the original chair.

You Try: Draw two valid chair conformations for each molecule shown below. Match the circled carbon to the circled carbon in the chair.

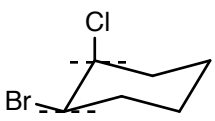


7. Be able to determine the *cis* or *trans* relationship between two substituents on a chair cyclohexane.

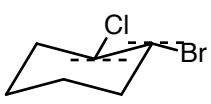
On the carbons containing the substituents of interest imagine or draw a horizontal line.
-If the two substituents are both above the line or both below the line, they are *cis*.
-If one substituent is above the line and one is below the line, they are *trans*.



cis - both Cl and Br are above the line.

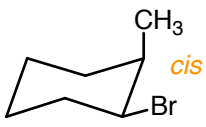


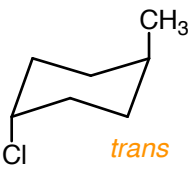
cis - both Cl and Br are above the line.



trans - Cl above and Br below.

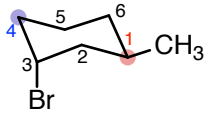
You Try: Identify each as *cis* or *trans.*



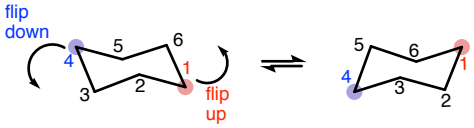


8. Be able to draw the ring flip conformation for a given chair containing multiple substituents.

a. Number the carbons on your chair. It may also be helpful to add reference points (the red circle at C1 and the blue circle at C4).

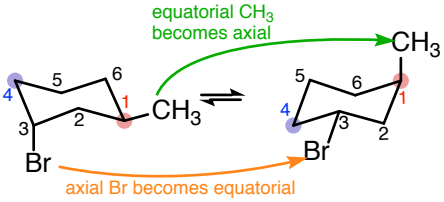


b. Flip one side up and the other side down to get the other chair structure.

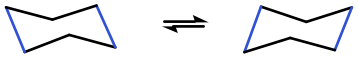


c. Place substituents. Keep them on the same numbered carbons.

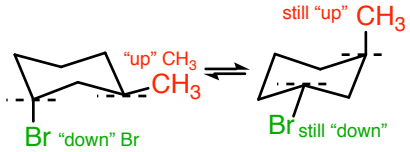
After a ring flip:
-Axial substituents become equatorial
-Equatorial substituents become axial



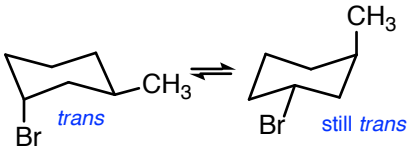
Some important things to note:



The side bonds in each ring flip conformer are angled in opposite directions.

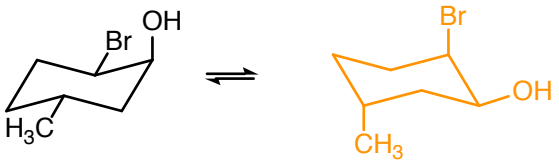


The directionality ("up" or "down") of groups does not change during a ring flip.



cis/trans relationships should not change

You Try: Draw the ring flip conformer for each chair below.



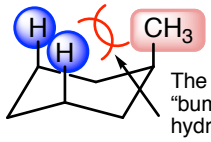
9. Be able to assess the relative stability of the two chair conformations for a given molecule.

-Having more groups equatorial increases stability.
-Having bulkier groups equatorial increases stability.

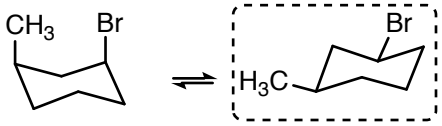
*A ring flip can move a bulky group from the axial orientation to the more stable equatorial orientation.

Compare the ring flip conformations in the two examples below.

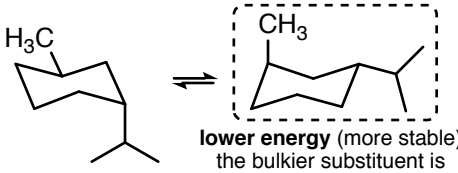
Bulky groups in the axial orientation suffer from unfavorable 1,3-diaxial interactions.



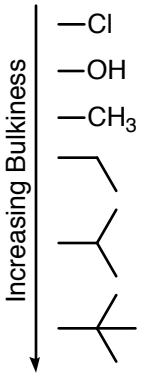
The bulky axial methyl group is "bumping" into the axial hydrogen that are 3-carbons away from the methyl.



lower energy (more stable) both substituents equatorial



lower energy (more stable) the bulkier substituent is equatorial



A substituent further down will have a larger energy cost (instability) associated with the axial orientation.

You Try: Draw the ring flip conformer and circle the one that is most stable.