

## Professor M. Wills.

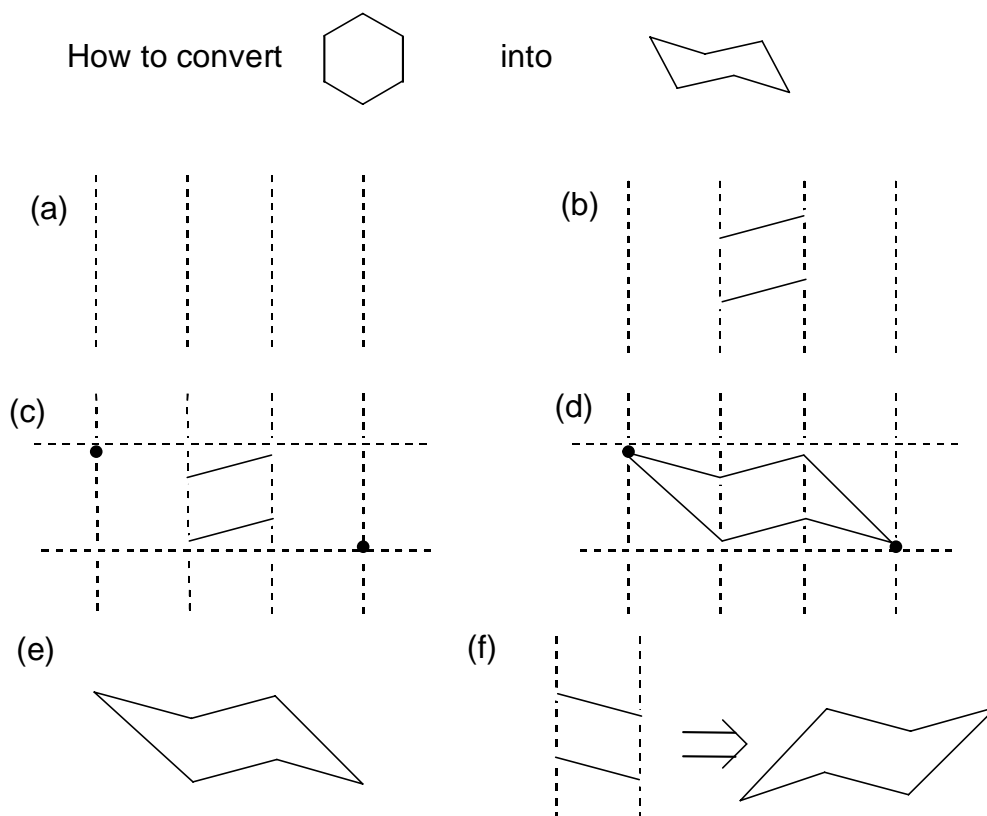
### How to draw a cyclohexane in 3D:

Six membered hydrocarbon rings often have a strong preference for 'chair' conformations because this puts all the substituents into positions where they bisect the adjacent groups (staggered conformation). This makes them very popular in exams about 3D structures of molecules. It also has an important effect on their reactivity.

Follow this process for help on drawing them, if you require it:

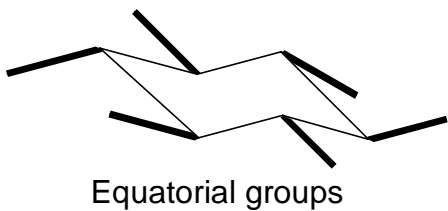
#### 1) Drawing the ring itself:

- First draw 4 thin parallel lines, ideally in light pencil.
- Then draw two parallel lines in the centre as shown, in normal strength.
- Next draw two dots, each in line with the top and lower extremities of the lines drawn in (b).
- Now join the dots to the lines in the middle as shown.
- Rub off the thin dotted lines you first drew and you are left with a 3D depiction of the cyclohexane chair structure.
- Drawing the two lines (in (b)) differently gives you the ring flip isomer.

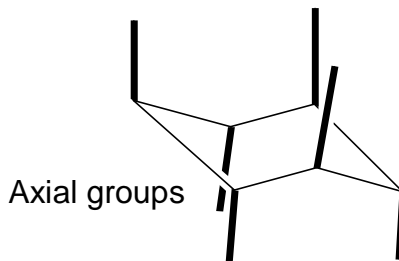
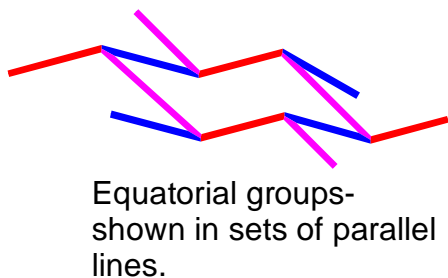


#### 2) Addition of equatorial and axial groups.

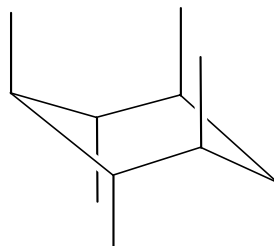
The substituents can be equatorial (projecting outward from the 'equator' of the molecule) or axial (sticking up and down parallel to the 'axis' of the molecule).



Hint - notice how the equatorial groups are parallel to the bond ONE C away in the ring:



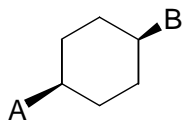
Hint: with practice, you might modify your original ring slightly to avoid overlaps:



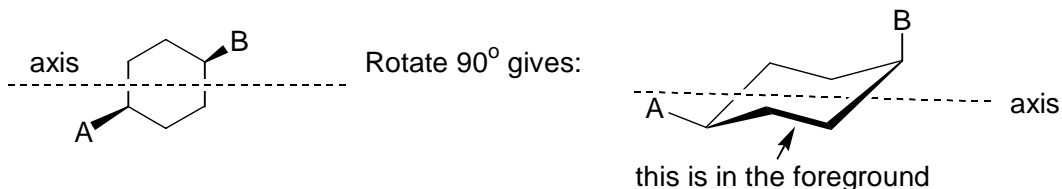
### 3) Change of perspective from 'hexagon' to 'chair' views.

Note how the perspective work here:

In the 'hexagon' diagram you are looking down from above the molecule:

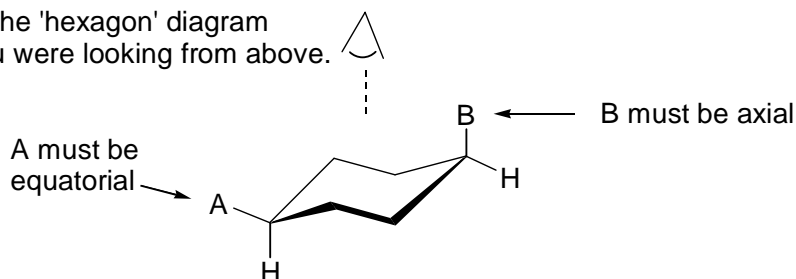


In the '3D' diagram you are looking 'side-on' to the molecule. You go from one to the other by turning the structure through 90 degrees along a horizontal axis:



Your old viewpoint (from above) is shown below:

In the 'hexagon' diagram you were looking from above.



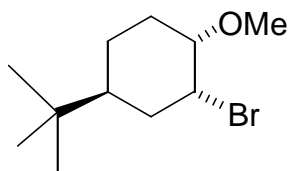
Notice how the 'B' group is *closer* to your previous viewpoint than the 'H' on the same C. This mean it *must* occupy an axial position, since the axial position is closer to your viewpoint than the equatorial one.

For the 'A' substituent, essentially the reverse is true, and the group is equatorial, i.e. the equatorial position is closer to your viewpoint than the axial, hence the group 'A' is equatorial.

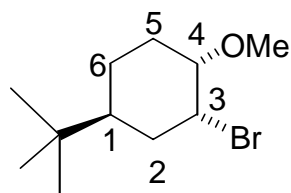
#### 4) Addition of substituents to equatorial and axial positions.

Now how to use the transfer of the perspective to the drawing of chair conformation rings with substituents at particular positions:

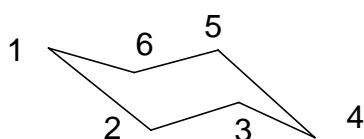
e.g. let's say you are given this molecule to draw in 3D:



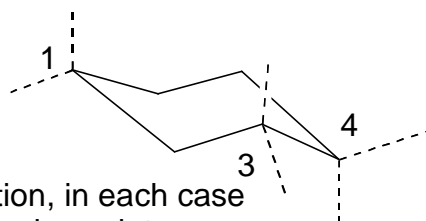
(a) put numbers on the Cs:



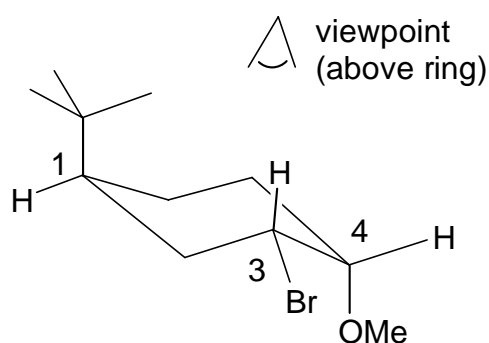
(b) draw a chair (either ring flip) and number the C atoms:



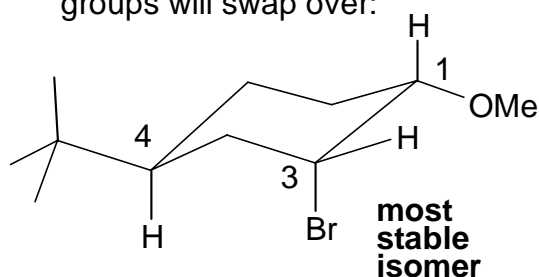
(c) lightly draw the positions of the equatorial and axial bonds to the substituents (but only on the Cs with groups attached):



(d) Add the substituents at each position, in each case judge whether they are closer to your viewpoint or further away, than the H also at that position:



(e) Repeat the process starting from the 'ringflip' isomer - all the axial/equatorial groups will swap over:



These are the two conformers you can form  
The most stable usually has the largest group (tBu) equatorial in order to avoid trans-diaxial interactions.

#### 5) Ring flip – note how all axial substituents go equatorial and vice versa when you 'ring flip':

