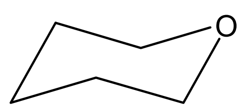
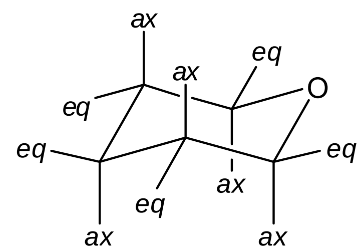
Chemistry 2301

Workshop 8 Solutions
Cyclohexane Conformers, and Sweetness

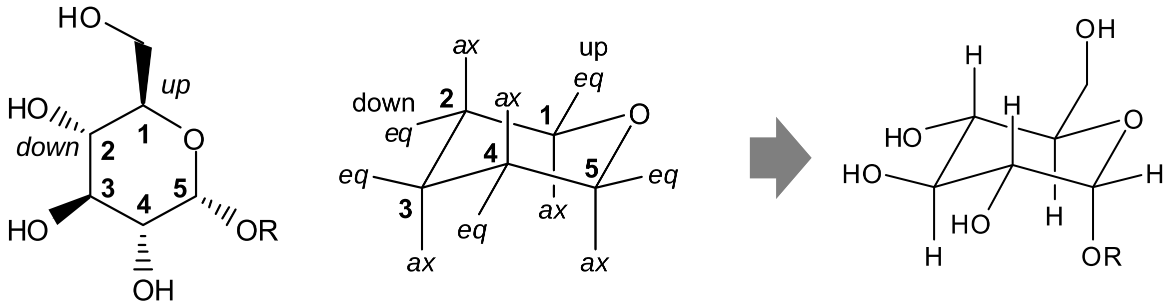
a) The first step in this problem is to draw equatorial and axial sticks on the cyclohexane chair, so we can then add substituents:



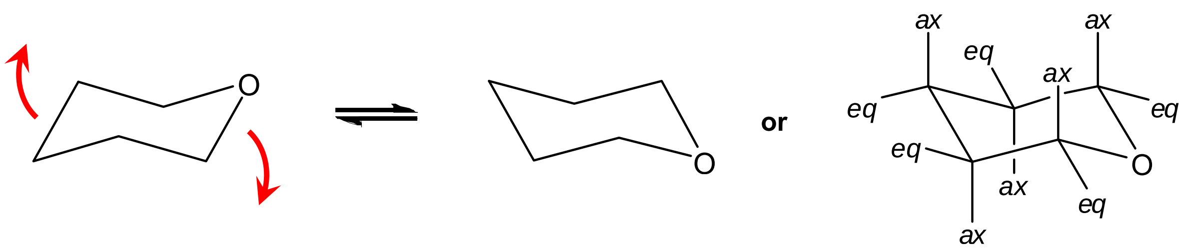
becomes



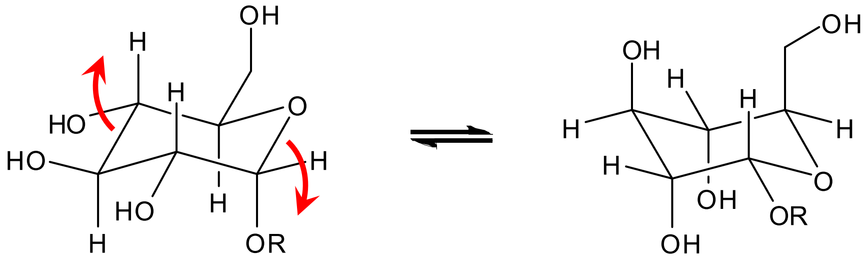
As you look around the ring, sometimes an equatorial stick is above an axial one, and sometimes an axial stick is above an equatorial one. That means that there isn't a direct relationship between "up" and either "axial" or "equatorial". But we can map the two-dimensional drawing—with its "up" wedges and "down" hashes—onto this axial/equatorial system on our 3-D drawing.



Now, we can flip the chair by pushing the oxygen down and the opposite end up:



When we flip a cyclohexane chair, all axial susbtituents become equatorial, and all equatorial substituents become axial. So,

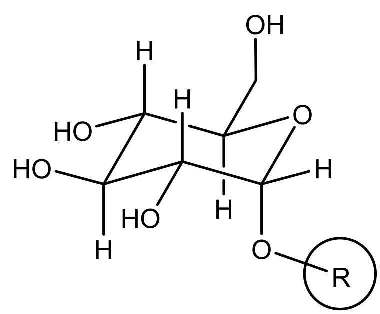


(our first chair)

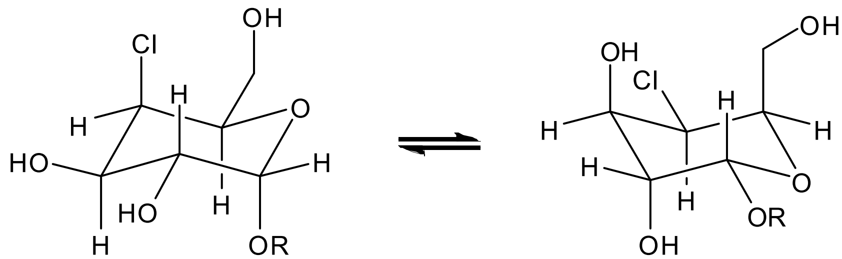
Note that the “up”-“down” relationships don’t change—substituents that were “up”—above the ring—are still “up”, and those that were “down” are still “down”.

b) Equatorial substituents are always more stable than axial ones. Looking at the two chairs above, the chair on the left has 4 equatorial and 1 axial substituent, while the chair on the right has 4 axial and 1 equatorial substituent. The chair with the fewest axial substituents—the one on the left—could be the most stable.

Of course, there is also a counter-argument to this. Out of the five substituents, the -OR group is the biggest. Maybe putting the biggest group equatorial outweighs the value of having the other four equatorial. I’m not sure about this, because the C-O bond in the –OR group can twist to point it’s “R” away from the rest of the ring, avoiding steric interactions:



c)

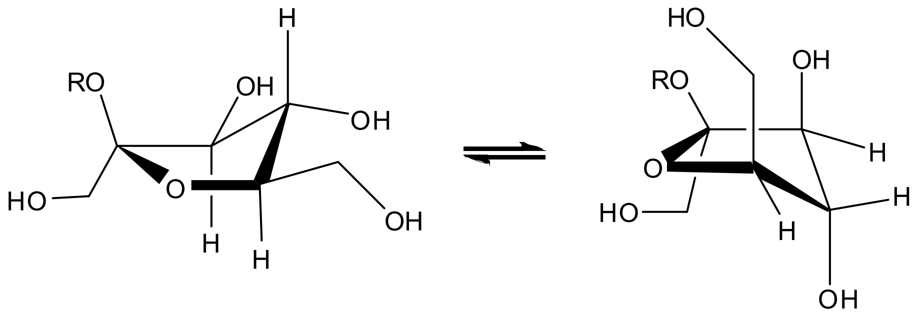


3 equatorial, 2 axial

2 equatorial, 3 axial

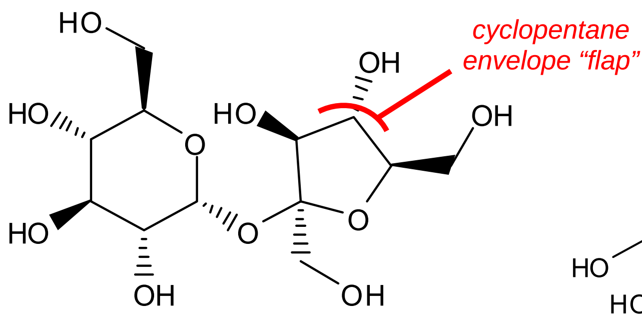
Again, I'd bet on the left conformer being more stable, with its –OR group pointed away from the rest of the molecule..

d)

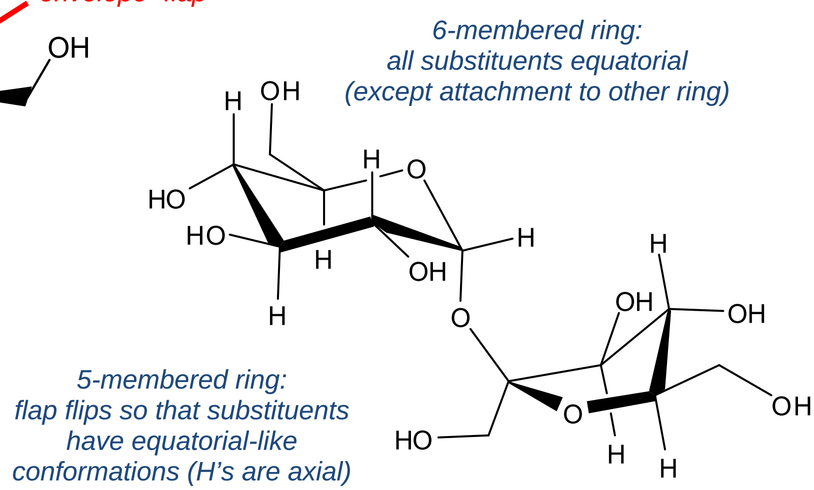


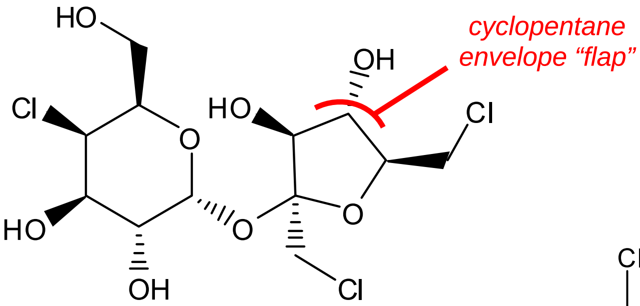
The left envelope has three equatorial-like substituents on the flap, so it would be more stable.

So, you could put this all together to construct the absolute most stable conformers of the two molecules:

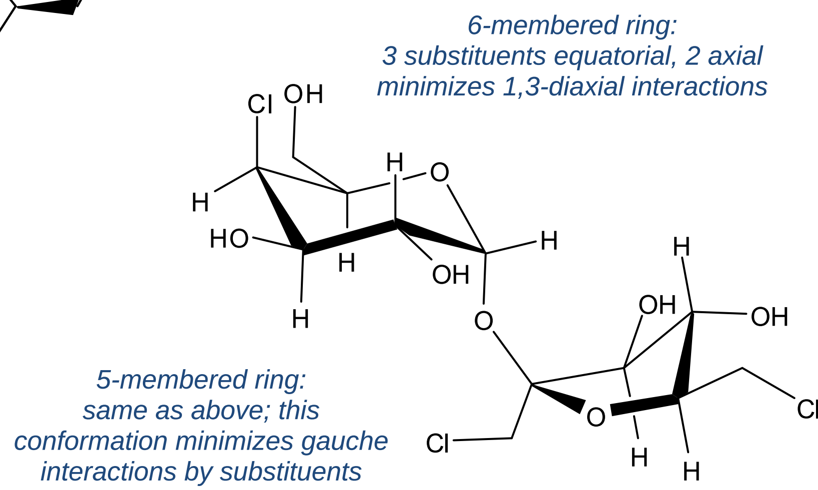


sucrose




HO
Cl
HO
OH
O
HO
OH
O
O
Cl
Cl
cyclopentane
envelope “flap”

sucralose


6-membered ring:
3 substituents equatorial, 2 axial
minimizes 1,3-diaxial interactions
5-membered ring:
same as above; this
conformation minimizes gauche
interactions by substituents
Cl
OH
H
O
H
HO
H
OH
H
H
O
H
OH
OH
Cl
O
Cl
H
H