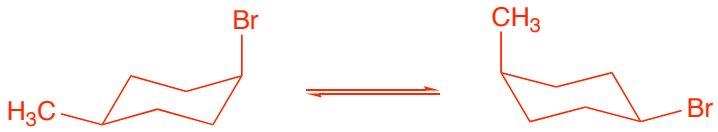
Chem 2061 Fall 2005 Name _____
Ch 3 Assignment
Due Friday, September 23

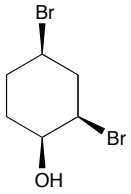
1. Draw the two chair conformations for each of the following substituted cyclohexanes. Use Wade table 3-6 to determine which of your conformations is more stable. Briefly explain why.

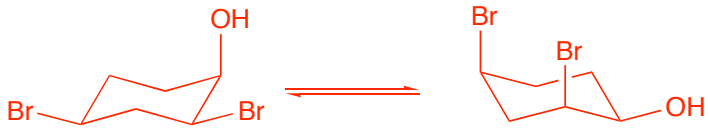
   a. *cis*-1-bromo-4-methylcyclohexane



ΔG(axial-equatorial) for bromocyclohexane is 0.6 kcal/mol while for methylcyclohexane it's 1.8. The larger value for methylcyclohexane indicates the methyl group has stronger and more unfavorable diaxial interactions than the bromine. Therefore the methyl group should be equatorial and the bromine axial in the more stable conformation, as in the left chair above.

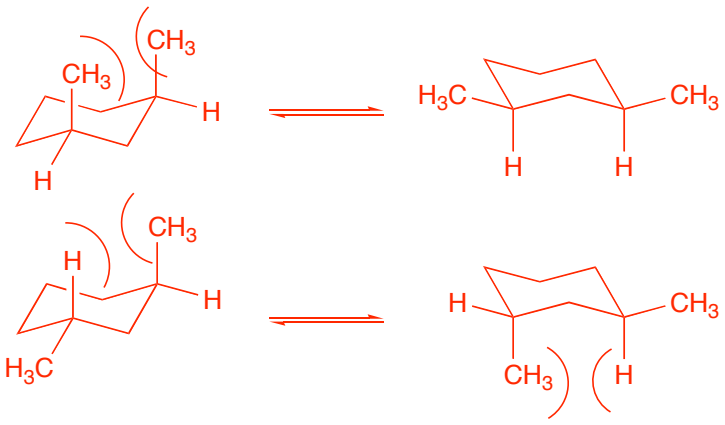
   b.





In this compound the ΔG in the table is slightly larger for an OH group than a Br, but the two cis axial bromines in the second chair will have a severly unfavorable diaxial interaction between each other. The first chair with the OH group axial will be more stable.

2. Which is more stable ***overall***, *cis*-1,3-dimethylcyclohexane or *trans*-1,3-dimethylcyclohexane? Why?



The *cis* compound has one conformation with both methyls axial, and another where both methyls are equatorial.

The *trans* compound has two equal-energy conformations with one axial methyl and one equatorial methyl.

The *cis* compound is lower in energy *overall* because there is a chair conformation with *no* diaxial interactions - with both the methyl groups equatorial. This one conformation will be lower in energy than either of the two equal *trans* conformations.