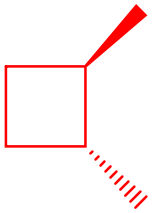
Discussion Worksheet #3 Partial Answers
Cycloalkanes and Cyclohexane Conformations

Skill 1: Nomenclature of cycloalkanes

- Name the parent chain "cyclo-"
- Number to give substituents lowest possible numbers
  - If tie, go alphabetically
- Name a cyclic substituent "cycloalkyl"
- Know "cis/trans" nomenclature

Problem 1. Draw these compounds:

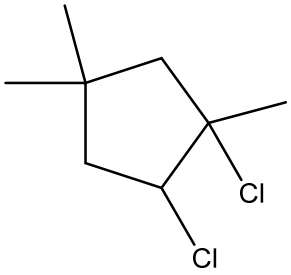
A. *trans*-1,2-dimethylcyclobutane



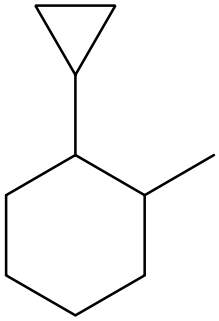
B. 1,1,4-trichlorocyclohexane

C. 1-cyclobutyl-2-isopropylcyclooctane

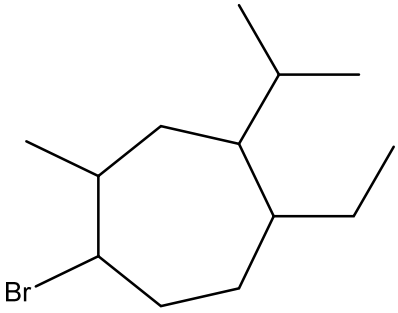
Problem 2: Name these compounds using systematic nomenclature



1,2-dichloro-1,4,4-trimethylcyclopentane



1-cyclopropyl-2-methylcyclohexane

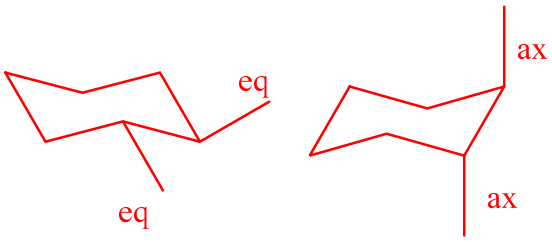


Skill 2: Drawing cyclohexane chair structures

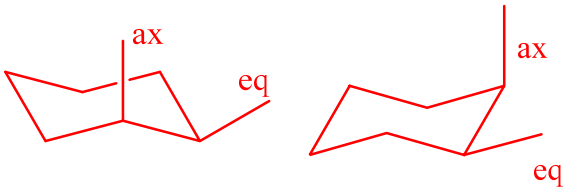
- Practice drawing chair and boat structures from flat structures, and vice versa
- Know the difference between "axial/equatorial" and "up/down" substituents
- Be able to draw a "chair flip" structure

Problem 3. Draw two chair structures for each of these compounds. Label each substituent as axial or equatorial.

A. trans-1,2-dimethylcyclohexane

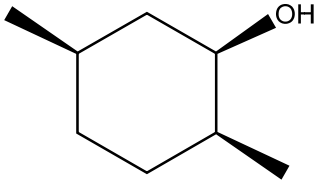
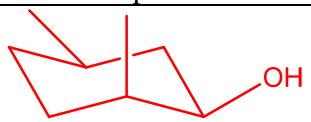
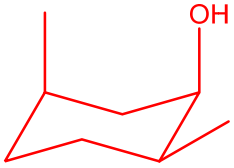
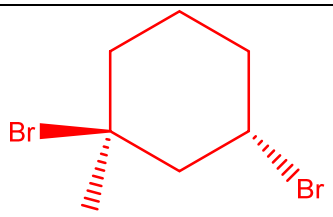
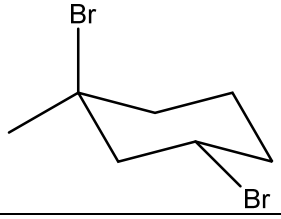
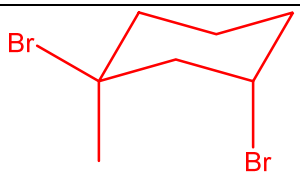


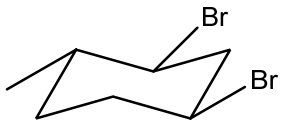
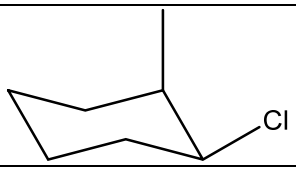
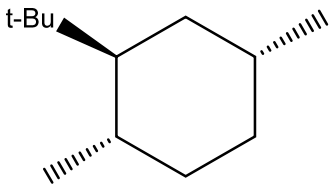
B. cis-1,2-dimethylcyclohexane



C. trans-1,3-dimethylcyclohexane

Problem 4. Fill in the chart below:

"Flat" structure	chair flip 1	chair flip 2
A. 		
B. 		

C.		
D.		
E. 		

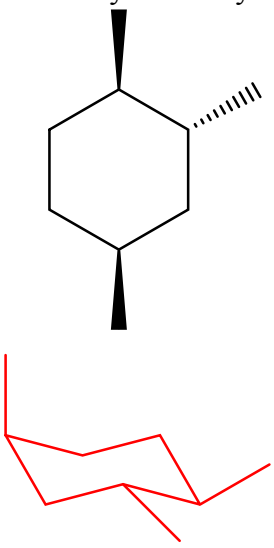
Skill 3: Relative stability of chair conformations.

- Substituents in the equatorial position are generally more stable than in the axial position due to torsional strain and gauche interactions (1,3-diaxial interactions)
- Use Vollhardt Table 4.3 to quantitate chair stability

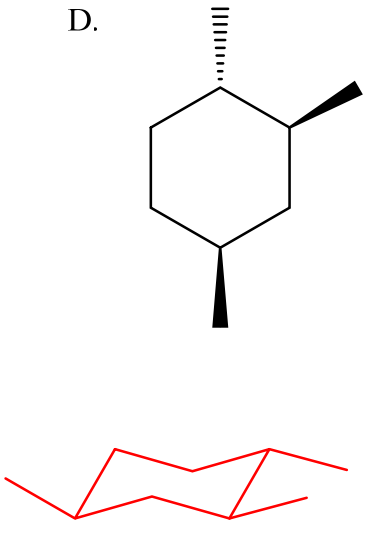
Problem 5. Draw the most stable chair structure for each of the following. If both are identical in energy, state so.

a. *trans*-1-t-butyl-4-methylcyclohexane
b. *cis*-1-t-butyl-4-methylcyclohexane

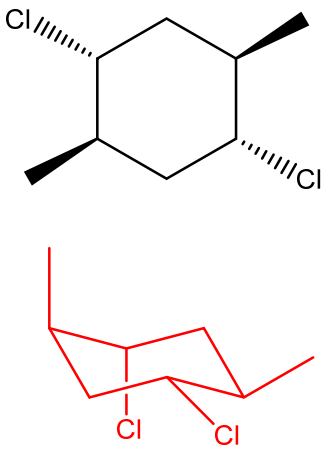
C.



D.



E.

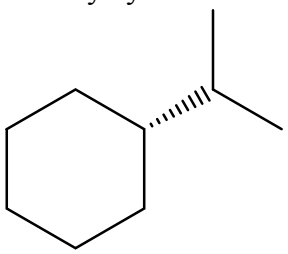


(other chair identical)

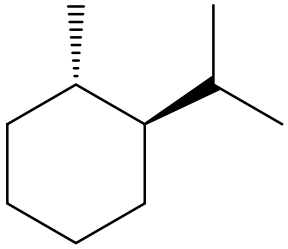
Problem 6. Calculate the difference in energy between the two chair conformations of each of these compounds. Use the thermodynamic rule of thumb to estimate a ratio of the two conformations.

a. *trans*-1-ethyl-2-methylcyclohexane
b. *cis*-1-ethyl-2-methylcyclohexane

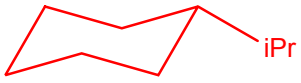
C.



D.



C.

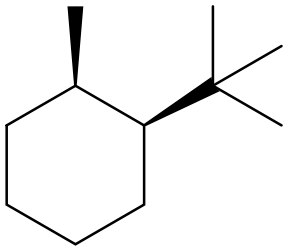


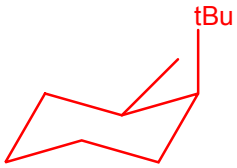
0 kcal

+ 2.2 kcal

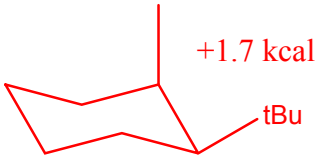
difference: 2.2 kcal--between 1.4 kcal and 2.8 kcal, so the ratio is between 1:10 and 1:100 in favor of the equatorial

E.





+ 5 kcal



difference: 3.3 kcal--between 2.8 and 4.2 kcal, so the ratio is between 1:100 and 1:1000 in favor of tBu equatorial. In other words, it is over 99% in that conformation