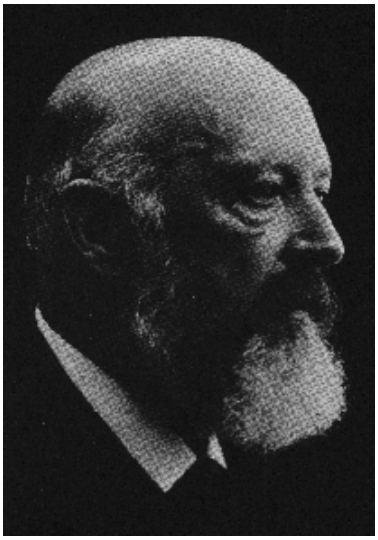
Chem 220a - Organic Chemistry

Problem Set 2

Chapter 3

Due: Monday, September 23, 2002



Adolf von Baeyer (1835-1917)

Baeyer's ideas on Strain Theory predicted that cyclopentane was less strained than cyclohexane. Because there was only one cyclohexane carboxylic acid, he concluded that there could not be both an equatorial and axial isomer.
Equatorial is often misspelled. Witness the map from the New York Times (5/23/00)

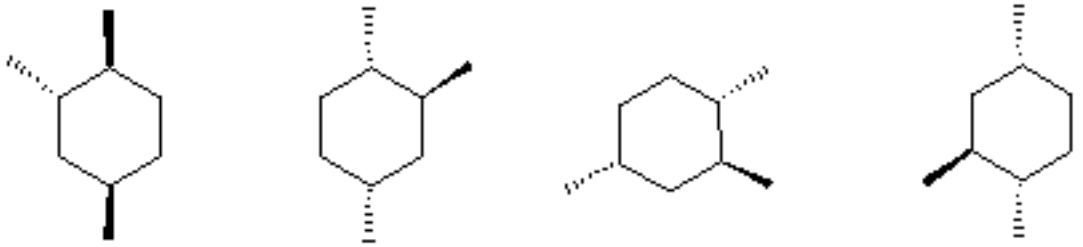
How to Draw Cyclohexanes (PowerPoint)

1. The Conformation Module in the Study Aids will give you a good overview of the subject of conformation. Work your way through it. (You will need Chime™ to view the Module). [How to manipulate Chime structures].

2. Redraw (line angle formula) and name (IUPAC) the hydrocarbon in this problem. For a dynamic view click here. For a static view click here. Get Chime™ here.

3. The $\Delta G^o = 0$ kcal/mol for the difference in energy between the two identical chair conformations of trans-1,3-dimethylcyclohexane. In what way, if any, do they differ? On the other hand, the energy difference between the two chair conformations of cis-1,2-dimethylcyclohexane is also $\Delta G^o = 0$ kcal/mol but they are isoenergetic (same energy) and not identical. In what way do they differ? [Note: Did you do #1?]

4. The four 1,2,4-trimethylcyclohexanes shown below are identical with one another.



1 **2** 3 **4**

a) Assemble a molecular model and convince yourself.

b) Imagine structure **1** at the origin of an xyz-axis system (x = horizontal, y = vertical, z = perpendicular to xy plane). What rotations are required to convert **1** into **2**? **1** into **3** ? **1** into **4**?

c) Determine ΔG^o for the difference in energy between the chair conformations of this 1,2,4-trimethylcyclohexane. Illustrate and explain.

5. Two 1,4-disubstituted cyclohexanes **A** and **B** are stereoisomeric. Compound **A** has an energy difference of 2.3 kcal/mol between its two chair conformations while compound **B** has a difference of 1.3 kcal/mol between its two chair conformations. What are the structures of **A** and **B**? Explain. [See pg. 118]

6. Determine the percentage of chair equatorial and axial isopropylcyclo**hexane** present at 25 ^oC. [$\Delta G^o = -RTlnK_{eq}$; R = 1.98 cal/mol-deg K. There are three staggered rotamers of the isopropyl group within the equatorial isomer. Assume that CH_3/CH_2 staggered = 0.9 kcal/mol , what is the energy difference between the two (two of them are isoenergetic)? Show calculations and illustrate.