

Fall Workshop #5

Question #1

A number of compounds can be drawn that contain two six-membered rings. They have the following molecular formulas:

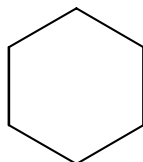
- (a) $C_{12}H_{22}$
- (b) $C_{11}H_{20}$
- (c) $C_{10}H_{18}$
- (d) C_8H_{14}

- For each molecular formula, build a model using your model kit that shows each structure containing the two cyclohexyl rings.
- Confirm the molecular formula using the degree of unsaturation (U) formula
- Find examples of primary, secondary, tertiary, and quaternary carbons.
- How many signals would be displayed in the ^{13}C -NMR spectrum for each compound above (see section 2.14 from your text)? Explain.
- Classify each ring system as “independent”, “spiro”, “fused”, and “bridged”.

Question #2

This question is designed to test your ability to draw accurate structures, build appropriate hand-held models, and derive qualitative and quantitative information for the following molecule: ***cis*-1-ethyl-4-methylcyclohexane**

- (a) Draw an accurate FLAT RING structure for the compound above using the template provided.



- (b) Build the molecule using your hand-held molecular modeling kit and then draw accurate CHAIR structures for BOTH chair conformations using the templates provided.

More stable conformer

Less stable conformer



- (c) Estimate (calculate) the potential energy for BOTH chair conformations using the table of potential energy interactions listed below.

type of interaction	energy (kcal/mol)
H to H torsional	0.9
H to CH ₃ 1,3-diaxial	1.3
CH ₃ to CH ₃ 1,3-diaxial	2.4
H to CH ₂ CH ₃ 1,3-diaxial	1.6
CH ₃ to CH ₃ gauche	0.9
CH ₃ to CH ₂ CH ₃ 1,3-diaxial	2.9
CH ₃ to CH ₂ CH ₃ gauche	1.4
CH ₂ CH ₃ to CH ₂ CH ₃ 1,3-diaxial	3.6

Potential energy (Chair conformation #1 – more stable) =

Potential energy (Chair conformation #2 – less stable) =

- (d) Consider the fact that the two chair conformations can be interconverted by a conformational ring flip. Find ΔH for the interconversion from MOST stable to LEAST stable and use that value to calculate K_{eq} . Assume that the reaction occurs at 35 °C, that $R = 8.314 \text{ J/mol K}$, and that $1 \text{ cal} = 4.184 \text{ J}$.

- (e) Discuss your calculated results and explain why they do or do not make sense.

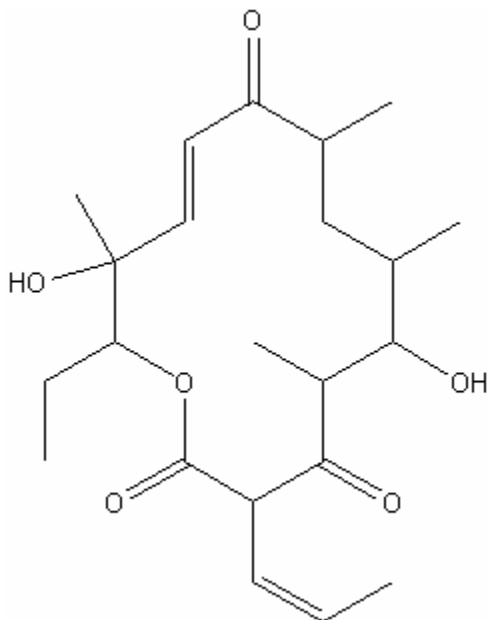
Question #3

Each person in the group should select one of the following compounds and repeat the directives in question #2. Be sure to *share your findings* with the group before going on.

- trans*-1-ethyl-4-methylcyclohexane**
- cis*-1-ethyl-3-methylcyclohexane**
- trans*-1-ethyl-3-methylcyclohexane**
- cis*-1-ethyl-2-methylcyclohexane**
- trans*-1-ethyl-2-methylcyclohexane**

Question #4

By definition, an asymmetric atom is any atom that has four DIFFERENT groups attached to it. Circle all of the **asymmetric carbons** in the following molecule, a derivative of the popular antibiotic, erythromycin A. In addition, draw a *star/asterisk* next to any **stereocenters** that do not contain asymmetric carbons (e.g. sites where you can get E/Z geometric isomerism). When finished, calculate the total number of stereoisomers that exist for this compound based upon the number of stereocenters that you found in the molecule.



Question #5

Each member of the workshop should build a model of **2-pentanol** using your handheld model kit. Draw a skeletal structure that is consistent with the model that you just built. Each person should assign the configuration (either R or S) to the molecule and then take turns comparing it to others in the workshop in terms of mirror imaging, superimposability, and stereochemical relationship (identical or enantiomers). Be sure to perform ALL possible comparisons just like we did in class!

Question #6

Repeat question #5, but now compare the various isomers of **3-bromo-3-methyl-2-pentanol** using your handheld model kit. Each person should assign the configuration (either RR, RS, SR, or SS) to the molecule and then take turns comparing it to others in the workshop in terms of mirror imaging, superimposability, and stereochemical relationship (identical, enantiomers, or diastereomers). Be sure to perform ALL possible comparisons just like we did in class!

Question #7

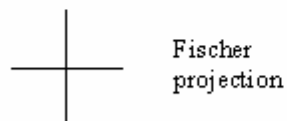
The general method for assessing stereochemical molecules is as follows:

- build the molecule
- assign R/S configuration
- perform superimposability/mirror image tests
- define relationships (see below)

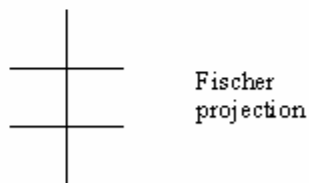
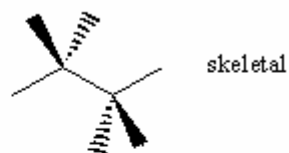
Possible relationships include:

- identical** -- completely superimposable non-mirror images
- enantiomers** -- non-superimposable, mirror images
- diastereomers** -- non-superimposable, non-mirror images
- meso** -- looks initially like a pair of enantiomers, but by virtue of an internal mirror plane, becomes superimposable

For a single stereogenic atom



For two stereogenic atoms



For more information on **Fischer projections**, see Figure 23.5 of the Jones text (remember that horizontal bonds are coming toward you and vertical bonds are going away from you).

Name each of the following structures (you'll need to build to assign R/S configuration) and then determine all isomeric relationships **among the first three** structures using the guidelines above.

