Fall 2004
Workshop #3

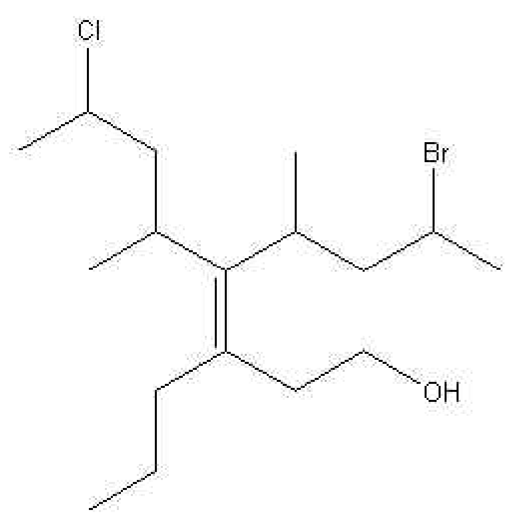
Question #1
An experimental technique called ^{13}C Nuclear Magnetic Resonance Spectroscopy allows chemists to tell how many different kinds of carbons there are in a molecule and whether carbons are primary (1°), secondary (2°), tertiary (3°), or quaternary (4°). Give **skeletal structures and names** for the following compounds having a molecular formula, C_6H_{12}. Also, on each structure, identify carbons as 1°, 2°, 3°, or 4°; tell how many different kinds of carbons there are; and designate which carbons are equivalent. Think seriously about connectivity and symmetry.

(a) A compound having only single bonds and only secondary carbons.
(b) A compound having only single bonds and primary, secondary, and tertiary carbons.
(c) A compound having only single bonds and only primary, secondary, and quaternary carbons.
(d) A compound having only single bonds and primary, secondary, tertiary, and quaternary carbons.
(e) For each compound in a-c, determine the number of distinct peaks you would observe in the molecule's ^{13}C-NMR spectrum.

Question #2
Draw isomers of C_9H_{20} that conform to each of the following restrictions. Be sure to name them according to the systematic nomenclature (IUPAC) that we introduced in class.

- An isomer that contains **only** an isopropyl group
- An isomer that contains **only** a t-butyl group
- An isomer that contains four methyl groups and has 5 peaks in its ^{13}C-NMR spectrum
- Also, give the structure of a C_8H_{18} compound that gives **only one** $C_8H_{17}Cl$ derivative.
- Draw the mono-chloro $C_8H_{17}Cl$ derivative and name it.

Question #3
Review the Cahn-Ingold-Prelog rules (Section 3.5 of your Jones text) for determining the E vs. Z designation for geometric alkene isomers with the other members of your group. Once you have reached a consensus, determine whether the following compound would be designated E or Z. Be prepared to explain your reasoning.



Question #4

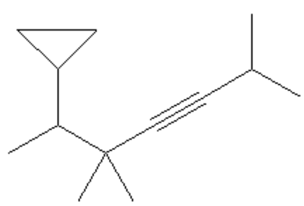
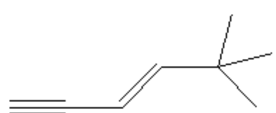
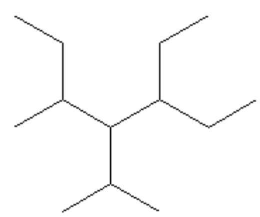
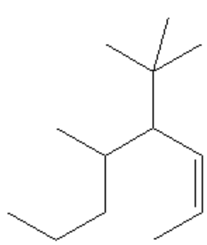
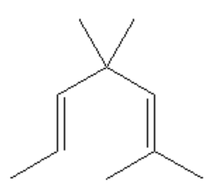
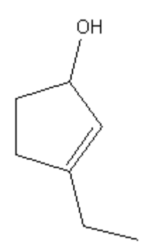
Draw structures for each of the following named compounds. *If the compound is not named properly, correct it.*

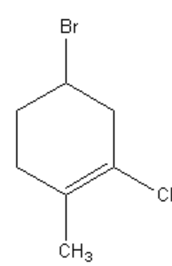
a. 3-ethyl-1-hexene (why do you not need to worry about E/Z designation here?)
b. (Z)-3,4,5-trimethyl-2-hexene
c. 4-methyl-2-pentyne
d. 1-cyclopropyl-3,4-dimethylcyclohexane
e. 2,5-dimethyl-4-tert-butylheptane
f. (E)-3-isopropyl-3-hexen-1-yne
g. 6-methylcycloheptene
h. 1-bromo-2-allyl-3-cyclopentene (refer to page 108 of your text)
i. (2E,6Z)-4-isobutyl-3-methyl-4-propyl-2,6-octadiene

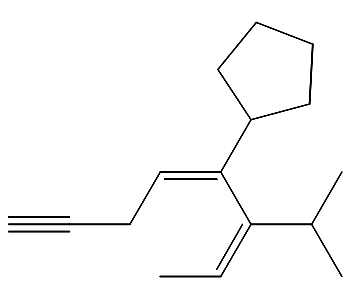
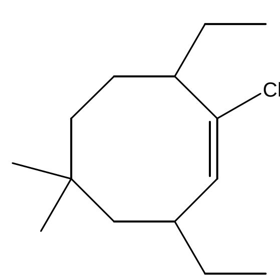
Question #5

In round-robin fashion according to the steps below, name each of the following compounds.

a. What is the base name/parent name for the molecule? How did you determine it?
b. What is the correct numbering pattern for the molecule? Why did you number it that way?
c. What are the substituents and at what number position are they located?
d. Do you have to worry about E/Z stereochemistry? Why or why not?
e. What is the full IUPAC name of the molecule?



Question #7

Using your model kit, build the following compound:

3-methylpentane

In round-robin fashion:

(a) locate the C_2-C_3 bond, and rotate so that the methyl group on C_2 and the ethyl group on C_3 are eclipsed (dihedral angle will be 0 degrees between these two groups)

(b) viewing down that bond, draw the Newman projection that you see

(c) find all eclipsing and gauche interactions – be sure to determine whether each interaction is the result of steric strain, torsional strain, or both

(d) using the data table below, calculate the energy for each interaction from part (c)

(e) plot the energy data point on a graph of energy (y-axis) as a function of dihedral angle (x-axis) with the following x-axis points = 0, 60, 120, 180, 240, 300, and 360 degrees

(f) rotate the **front half** of the molecule around C_2-C_3 by 60° to the **right** to generate a new conformation

(g) repeat steps (b) through (f) until you completed a full 360° rotation

Interaction	**Energy (kcal/mol)**
CH_3-CH_3 gauche	0.6
CH_3-H eclipsing	1.6
CH_3-CH_3 eclipsing	2.6
CH_3-CH_3CH_2 gauche	0.9
CH_3CH_2-H eclipsing	1.8
H-H eclipsing	0.9
CH_3-CH_3CH_2 eclipsing	3.1