Organic Chemistry CH 352-02 (Wilson)

Exam #1

February 17, 1998

Question 1 _______ (10)
Question 2 _______ (15)
Question 3 _______ (9)
Question 4 _______ (15)
Question 5 _______ (20)
Question 6 _______ (21)
Question 7 _______ (10)
E.C. _______ (4)

TOTAL _______ (100)

"When the going gets weird, the weird turn pro."    -Hunter S. Thompson
1. Draw the all the molecular orbitals for the methyl-allyl anion \([\text{CH}_2\text{C(CH}_3\text{)}\text{CH}_2^-]\). Include all the bonding, non-bonding, and anti bonding orbitals, as appropriate. Draw the molecular orbital diagram and fill in the MO's with the appropriate number of electrons.

2. Choose one of the following equations and give the mechanism for the reaction. Be sure to include all important intermediates and use "arrow pushing" to show the flow of electrons. Credit will be given for only one mechanism.

\[
\text{O} - \text{I} \text{ (excess)} \xrightarrow{\text{DMSO}} \text{I} + \text{H}_2\text{O} \quad \text{OR} \quad \text{H} - \text{Me} \xrightarrow{\text{Na/NH}_3, -40 \degree \text{C}} \text{H} - \text{Me}
\]
3. Given the following "roadmap," give the appropriate structures for A, B and C. Be aware that small pieces may have been lost in a transformation and not shown!

\[
\begin{array}{ccc}
\text{NC} & \text{Br}_2 & \text{A} \\
\text{C}_4\text{H}_2\text{N}_2\text{Br}_2 & \text{KOH} & \Delta & \text{B} \\
\text{C}_4\text{N}_2 & \text{H}_2, \text{Pd/BaSO}_4 & \text{quinoline} & \Delta & \text{C} \\
\text{C}_4\text{H}_2\text{N}_2 & \text{MeO} & \text{OMe} & \text{CN} & + \text{enantiomer}
\end{array}
\]

A =

B =

C =

4. Synthesize one of the following compounds. Legal starting materials include acetylene, bromobenzene, monofunctional alcohols of four carbons or less, and any inorganic reagent or solvent. Keep in mind, if carbons are added to a molecule, make sure those carbons come from a legal starting material! There are multiple correct answers to each compound and partial credit will be assigned to partial syntheses.

\[
\begin{array}{ccc}
\text{OR} & \text{CH}_3 & \text{OH} \\
\text{OR} & \text{C}_3\text{H}_5 & \text{OH} \\
\text{OR} & \text{OEt} & \text{OH}
\end{array}
\]
5. A compound has the molecular formula C\textsubscript{10}H\textsubscript{12}O\textsubscript{2} and the following IR, \textsuperscript{1}H NMR, and \textsuperscript{13}C NMR data. Use this information to answer the questions on the next page.

IR:

\textsuperscript{1}H NMR:

\textsuperscript{13}C NMR:
a. How many units of unsaturation does this molecule have? (3 pts.)

b. What feature(s) is(are) present in the IR that indicate functional group(s)? Be specific! (3 pts.)

c. What features about the $^1$H NMR spectrum indicate anything about functional groups or connectivity about the compound? (7 pts.)

d. What information, if any, does the $^{13}$C NMR spectrum give you? (4 pts)

e. What is the structure of the compound? (4 pts.)
6. Predict the product or products for four out of the next five reactions. Choose only four. Be mindful of details such as stereochemistry and regiochemistry.

a. 
\[
\text{\begin{align*}
\text{CH}_3\text{C} & \text{H} \\
\text{NaH}_2 & \text{H}_3\text{O}^+ \\
2,3\text{-epoxy-3-methylhexane} & \\
\end{align*}}
\]

b. 
\[
\text{\begin{align*}
\text{CH}_2=\text{CH}-\text{NMe}_2 & \text{CN} \\
\text{NMe}_2 & \text{CN} \\
\Delta & \\
\end{align*}}
\]

c. 
\[
\text{\begin{align*}
\text{Br} & \text{Br} \\
\text{Br} & \text{KOH, \Delta} \\
\text{HBSi}_2 & \\
\text{H}_2\text{O}, \text{KOH} & \\
\end{align*}}
\]

d. 
\[
\text{\begin{align*}
\text{C}_6\text{H}_5 & \text{CH}_2 \text{Cl}_2 \\
\text{H}^+ \text{isopropanol} & \\
\end{align*}}
\]

e. 
\[
\text{\begin{align*}
\text{CH}_2=\text{CH} & \text{OEt} \\
\text{CO}_2\text{Me} & \Delta \\
\end{align*}}
\]
Assistant Beaker has taken two IR's of esters that he made in the laboratory. One is of methyl salicylate (oil of wintergreen) and the other is of methyl octanoate. Both of the structures are shown below. Match the structure to the correct IR spectrum. Explain why you made your choices based on specific stretches (be detailed!!!).