Name _____________________________

ORGANIC CHEMISTRY CH 352-02 (Esteb)
Exam #2
February 28, 2002

Question 1 _________  (20)
Question 2 _________  (26)
Question 3 _________  (26)
Question 4 _________  (12)
Question 5 _________  (10)
Question 6 _________  (6)

E. C. _________  (3)

TOTAL _________  (100)

... AND THEN I HEARD A LOUD BANG AND WHEN I TURNED BACK HE WAS GONE!

COOL IT, GARY...
HERE COMES THE BOUNCER...

www.offthemark.com
1. Give product(s) for **four of the following five** reactions. Bear in mind things like regiochemistry, stereochemistry, etc. where appropriate. (5 pts each)

a) 
\[
\begin{align*}
\text{Br} & \\
\text{1)} \text{ KOEt, EtOH} \\
\text{2)} \text{ HBr, peroxides} \\
\text{3)} \text{(CH}_3\text{CH}_2\text{)}_2\text{CuLi}
\end{align*}
\]

b) 
\[
\begin{align*}
\text{OH} & \\
\text{1)} \text{ CH}_3\text{MgBr, Et}_2\text{O} \\
\text{2)} \text{ PhCH}_2\text{Br, THF}
\end{align*}
\]

c) 
\[
\begin{align*}
\text{1)} \text{ Cl} & \\
\text{2)} \text{ CH}_3\text{Li, Et}_2\text{O} \\
\text{3)} \text{ H}_3\text{O}^+, \text{ heat} \\
\text{4)} \text{ mCPBA, CH}_2\text{Cl}_2
\end{align*}
\]

d) 
\[
\begin{align*}
\text{Br} & \\
\text{1)} \text{ 2 Li, pentane} \\
\text{2)} \text{ 1/2 CuI, THF} \\
\text{3)} \text{ 1-iodobutane}
\end{align*}
\]

e) 
\[
\begin{align*}
\text{1)} \text{ CH}_2\text{I}_2, \text{ Zn/Cu} \\
\text{2)} \text{ PhMgBr, Et}_2\text{O} \\
\text{3)} \text{ H}_3\text{O}^+
\end{align*}
\]
2. Given that you have a compound with the following spectral data, answer the questions below:

Elemental composition is C: 79.96%, H: 9.39%
a. What is the empirical formula? (3 pts)

\[ C_{10}H_{14}O \]

b. What information did you get from the mass spectrum? (3 pts)

\[ M^+ = 150 \text{ and benzylic cleavage, also empirical = molecular formula} \]

c. How many units of unsaturation do you have? (2 pts)

\[ 10 + 1 - 14/2 = 4 \]

d. What information did you get from the IR spectrum? (4 pts)

OH stretch at 3350 = alcohol, \(sp^2\) C-H stretching at 3000+ and \(sp^3\) C-H stretching at 3000 and below, suspect 1600 and 1500 from benzene ring.

e. What information did you get from the \(^{13}\)C NMR spectrum? (4 pts)

Disubstituted aromatic ring with only 4 unique carbons. Peak at 65 suggests a CH\(_2\) group next to an electronegative atom (O). Presence of CH and CH\(_3\) groups at 32 and 22 ppm, respectively.

f. What information did you get from the \(^1\)H NMR spectrum? Include interpretation of details such as integration, coupling patterns, and chemical shifts (6 pts)

Para disubstituted benzene 2 doublets of 2H each
Doublet at 4.5 from CH\(_2\) group next to O.
Triplet at 3 is from OH adjacent to CH\(_2\) group
The 1H septet and 6H doublet is characteristic of an isopropyl group
g. What do you think the structure of the compound is? (4 pts)

(26) 3. Given that you have a compound with the following spectral data, answer the questions below:

Elemental composition is C: 51.72 %, H: 6.94 %
a. What is the empirical formula? (3 pts)

\[ C_5H_8O_3 \]

b. What information did you get from the mass spectrum? (3 pts)

\[ M^+ = 116, \text{emirical} = \text{molecular formula} \]

c. How many units of unsaturation do you have? (2 pts)

2

d. What information did you get from the IR spectrum? (4 pts)

3100 OH stretch probably from carboxylic acid
at least one carbonyl stretch at 1700

e. What information did you get from the \(^{13}\)C NMR spectrum? (4 pts)

2 carbonyls neither of which are an aldehyde
CH\(_2\), CH\(_2\), and CH\(_3\) groups are present

f. What information did you get from the \(^1\)H NMR spectrum? Include interpretation of
details such as integration, coupling patterns, and chemical shifts (6 pts)

Carboxylic acid confirmation at 11.5
The two triplet 2H, s suggest CH\(_2\)-CH\(_2\) pattern
The 3H singlet suggests CH\(_3\) group not adjacent to any proton bearing atoms i.e. one of
the carbonyls
The CH\(_2\)-CH\(_2\) must be in between two carbonyls since groups cannot contain any
protons

g. What do you think the structure of the compound is? (4 pts)

\[
\begin{align*}
\text{HO} & \quad \text{CH}_2-C\text{H}_3 \\
\text{C} & \quad \text{C} \\
\end{align*}
\]
4. Synthesize one of the following two compounds using reasonable, high-yield synthetic steps. Your legal starting materials are benzene, monofunctional compounds of 4 carbons or less – but not organometallic compounds (you have to make those), inorganic reagents (mCPBA, NBS, Mg, etc.), and solvents. (12 pts each)

Any reasonable synthesis accepted. Come see me if you have questions.

5. Provide a detailed arrow pushing mechanism for the following transformations. (5 pts each)
6. Circle the correct answer for the following 3 questions. (2 pts each)

a) The following MS is of an alkyl bromide M+ and M+2 peak same height. Also loss of 79.

b) This compound will have a larger lambda max in its UV spectrum.

This one is more conjugated hence higher number
c) This compound will have four negative DEPT signals.

\[ \text{or} \]

The middle compound contains 4 CH\textsubscript{2} groups. CH\textsubscript{2} groups show up as negative peaks.

(3) Extra Credit:

Name any Olympic event that the U.S. won a gold medal in during the 2002 Winter Olympics.

See me for a complete list