Chem 334, Exam 2
Professor Fox
Spring 2009

Your Name

Your TA's Name

Question 1, 3 points each
Question 2, 12 points
Question 3, 12 points
Question 4a, 10 points
Question 4b, 10 points
Question 4c, 10 points
Question 4d, 10 points
Question 4e, 18 points
1. Match the following compounds with their $^{13}$C NMR spectra. Note: only chemical shift data is given [multiplicities (s,d,t,q) are not needed to solve this problem]

- **A**: N=C
- **B**: CH$_3$
- **C**: OCH$_3$
- **D**: H=O
- **E**: OH
- **F**: OH

**Note**: * = 2 carbons
2. Explain how you would use $^1$H NMR spectroscopy to distinguish the following compounds. You may use chemical structures to support your answer, but use no more than 30 words.

**Trans Alkene:** expect $J \approx 17$ Hz

**Cis Alkene:** expect $J \approx 10$ Hz

3. Explain how you would use IR spectroscopy to distinguish the following compounds. You may use chemical structures to support your answer, but use no more than 30 words.

**$\alpha,\beta$ Unsaturated Ketone:** expect $\approx 1685$ cm$^{-1}$

**Unconjugated Ketone:** expect $\approx 1715$ cm$^{-1}$
4. Elucidate the following structure

\[ \text{C}_{11}\text{H}_{12}\text{N}_{2}\text{O}_{2} \]

\begin{align*}
\text{\textsuperscript{13}C NMR} & & \text{\textsuperscript{1}H NMR} & & \text{IR (cm}^{-1}\text{)} \\
168.2 \text{ (s)} & & 8.0 \text{ (br s, 1H)} & & 3600-3300 \text{ (br)} \\
139.7 \text{ (s)} & & 7.57 \text{ (d, J=7.7 Hz, 2H)} & & 2260 \\
136.5 \text{ (s)} & & 7.17 \text{ (d, J=7.7 Hz, 2H)} & & 1690 \\
127.5 \text{ (d, 2 carbons)} & & 4.50 \text{ (dd, J=7.9, 6.5 Hz, 1H)} & & 1530 \\
120.5 \text{ (d, 2 carbons)} & & 2.89 \text{ (dd, J=7.9, 4.0 Hz, 1H)} & & \text{ (IR taken with dilute sample)} \\
117.7 \text{ (s)} & & 2.78 \text{ (dd, J=6.5, 4.0 Hz, 1H)} & & \text{ (IR taken with dilute sample)} \\
70.3 \text{ (d)} & & 2.02 \text{ (s, 3H)} & & \text{ (IR taken with dilute sample)} \\
28.0 \text{ (t)} & & 1.98 \text{ (bs, 1H)} & & \text{ (IR taken with dilute sample)} \\
17.6 \text{ (q)} & & \text{} & & \text{} \\
\end{align*}

(a) Circle the functional group that is associated with

- **Note:** "Ar" refers to aryl, or an aromatic ring

(i) IR: 2260 cm\(^{-1}\) and \textsuperscript{13}C NMR: 117.7 ppm (both spectral characteristics are associated with the same functional group)
4. Elucidate the following structure

b) Circle the functional group that is associated with

(note: "Ar" refers to aryl, or an aromatic ring)

(l) IR: 1690 and 1530 cm\(^{-1}\) and \(^{13}\)C NMR: 168.2 ppm (all 3 spectral characteristics are associated with the same functional group)

alkene  ether  alkyl chloride

alkyl alcohol amine

alky chloride

phenyl phenol

alkylketone mono-arylketone diarylketone

alkylketone alkylnitrite arylnitrite

alkyl alkylationdearyldehyde

alkylcarboxylic acid

alkylcarboxylic acid

alkylcarboxylic ester

alkylcarboxylic ester

nitro aromatic

secondary amide

lactam

alkyl acid chloride

aryl acid chloride

7.57 (d, J=7.7 Hz, 2H)

7.17 (d, J=7.7 Hz, 2H)

p-substituted benzene
d. Assign the following coupling constants. Your answer must clearly indicate which protons are coupled to one another.

4.50 (dd, J=7.9, 6.5 Hz, 1H)
2.89 (dd, J=7.9, 4.0 Hz, 1H)
2.78 (dd, J=6.5, 4.0 Hz, 1H)

e) draw the structure of the product (no partial credit)