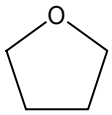
CHEM 2311
E6 practice-iv

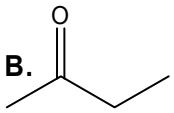
Tables of IR frequencies and ^{1}H and ^{13}C NMR shifts are attached
You may use a calculator on this exam

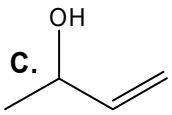
Atomic Masses: H, 1.01; C, 12.01; N, 14.00; O, 16.00;
Cl, 35.45 (a 3:1 ratio of ^{35}Cl and ^{37}Cl); Br, 79.90 (a 1:1 ratio of ^{79}Br and ^{81}Br)

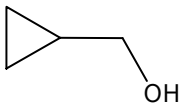
1. (32 points) Circle the letter *on the right* which corresponds to the answer to each question. There is only one correct answer for each question.

(i) Which of the following compounds gives an infrared spectrum with peaks at 3300 cm^{-1} (strong, broad peak) and 1640 cm^{-1} (sharp, weak peak), but no strong peak at approximately 1720 cm^{-1}?

A. 

B. 

C. 

D. 

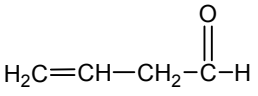
(ii) Which of the following is most consistent with a molecule having a molecular ion with *m/e* of 73?

E. the molecule contains bromine **F.** the molecule contains nitrogen
G. the molecule is an alcohol **H.** the molecule is an alkene

(iii) Which feature in the ^{1}H NMR spectrum provides information about the number of neighboring protons of each proton in the compound?

I.. number of signals **J.** integral
K. multiplicity **L.** chemical shift

(iv) Which of the protons in 3-butenal (shown at right) appear at furthest downfield in the ^{1}H NMR spectrum?



M. *i* **N.** *ii* **O.** *iii* **P.** *iv*

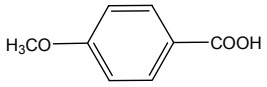
(v) What are products of the collision between high energy electrons and methane?

Q. $CH_4^- + 2\ e^-$ **R.** $CH_3^- + H^{\cdot}$
S. $CH_4^+ + 2\ e^-$ **T.** $CH_3^{\cdot} + H^+ + 2\ e^-$

(vi) Which of the following series of peaks appears in the ^{1}H NMR spectrum of 1,4-butanediol ($HOCH_2CH_2CH_2CH_2OH$)?

U. three singlets **V.** two triplets and a quartet
W. a singlet and two triplets **X.** a singlet, a triplet and a pentet

(vii) How many signals appear further downfield than 100ppm in the ^{13}C NMR spectrum of 4-methylbenzoic acid (shown at right)?



Y. 4 **Z.** 5 **AA.** 6 **BB.** 8

(viii) Which of the following gives a ^{13}C NMR spectrum consisting of 4 peaks?

CC. 2-methylpentane **DD.** 2,4-dimethylpentane
EE. 3,3-dimethylpentane **FF.** hexane

A B C D E F G H I J K L M N O P Q R S T U V W X Y Z AA BB CC DD EE FF

2. (26 points)

(i) (4 points each) Provide a single molecular structure consistent with the following data. The NMR data is complete. The IR spectra have a number of peaks, only the most relevant are provided.

Compound **A**: C_6H_6ClN

^{1}H NMR: δ 3.6 (singlet, 2H)
δ 6.6 (doublet, 2H)
δ 7.1 (doublet, 2H)

IR: 3520 (broad), 3400 (broad), 3050 cm^{-1} (and others)

Compound **B**: $C_6H_{11}ClO_2$

^{1}H NMR: δ 1.2 (singlet, 9H)
δ 4.1 (singlet, 2H)

IR: 1740, 1210 cm^{-1} (and others)

Compound **C**: C_4H_9ClO

^{1}H NMR: δ 2.1 (pentet, 2H)
δ 3.3 (singlet, 3H)
δ 3.4 (triplet, 2H)
δ 3.7 (triplet, 2H)

IR: peak at 1160 cm^{-1} (and others)

Compound **D**: C_3H_6O

^{1}H NMR: δ 2.7 (pentet, 2H)
δ 4.7 (triplet, 4H)

IR: peak at 1120 cm^{-1} (and others)

(ii) (5 points each) Compound **E** gives a combustion analysis of C 49.41%; H 6.83%

(a) What is the *empirical formula* of **E**?

(b) What is the value of SODAR for the *smallest possible molecular formula* of **E**?

3. (17 points) Refer to the data provided on the following page. *Note that you receive credit for each part of this answer, the structure you provide in part (n) is only worth 1 point. Each part is graded independently without reference to other answers*

Analysis of Combustion Analysis/Mass Spectrum

(a) What is the *molecular* formula? _____.

(b) What is the value of SODAR? _____.

Analysis of IR spectrum (in conjunction with formula)

(c) Which of the following are present? (circle all that are present)

O-H C-O C=O

Analysis of the ^{13}C NMR spectrum (in conjunction with IR and SODAR)

(d) How many different types of carbon atoms are there in the molecule:_____.

(e) How many different types of sp^3 carbon atoms are there in the molecule:_____.

(f) How many types of aromatic carbons are there?_____.

(g) What structural feature does the peak at 62 ppm suggest?_____.

Analysis of ^1H NMR spectrum (in conjunction with the formula and IR)

(h) How many different types of hydrogen atom are there in the molecule?_____.

(i) What is the ratio of the number of each type of proton, proceeding from left to right across the spectrum? (*i.e.*, 6:3:1)_____.

(j) Describe the multiplets (*i.e.*, s, d, t, q) at: δ 3.8 ppm _____, and δ 2.8 ppm _____.

(k) Which of the following are present? (circle all that are present)

Et iPr tBu vinylic H (i.e. an alkene) aromatic H

(l) How many aromatic hydrogens are there?_____.

(m) How many substituents are there on the benzene ring?_____.

Putting it all together

(n) Suggest a single structure for the molecule that is consistent with all of the data presented.