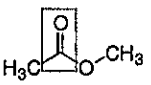
Spring 2012 2320 E1

I. **Theory**

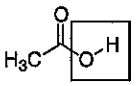
1. Complete each of the following equations by filling in the missing symbol. (4 points)

$\Delta E = h\nu$ $\qquad$ $\lambda = \frac{c}{\nu}$

2. Predict the IR absorption frequency within 20 wavenumbers for each of the indicated bonds. (4 points)



1740 cm^{-1}



3000 cm^{-1}

3. Circle all nuclei that have a nuclear spin? (4 points)

(a) $^{2}_{1}H$ b) $^{32}_{16}S$ (c) $^{31}_{15}P$ d) $^{56}_{26}Fe$ e) $^{24}_{12}Mg^{+}$

4. A ^{13}C NMR spectrum that features splitting of each carbon peak according to the number of hydrogens bound to each carbon is called _____. (2 points)

(a) off-resonance b) COSY c) FT d) DEPT e) HETCOR

5. The ____ region of the electromagnetic spectrum influences molecular vibrations. (2 points)

(a) IR b) UV c) visible d) radiowave e) microwave

6. Name two factors that influence the wavenumber in which a specific bond absorbs in IR spectroscopy. (4 points)

1) Mass of atoms in the bond

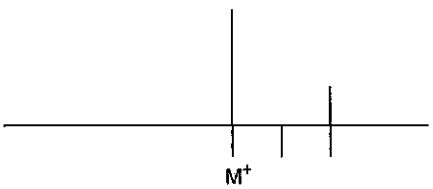
2) Bond strength

7. Tell what role a magnetic field plays in each of the following analytical methods. (4 points)

a) Mass Spectrometery: causes ions to bend flight path in the flight tube.

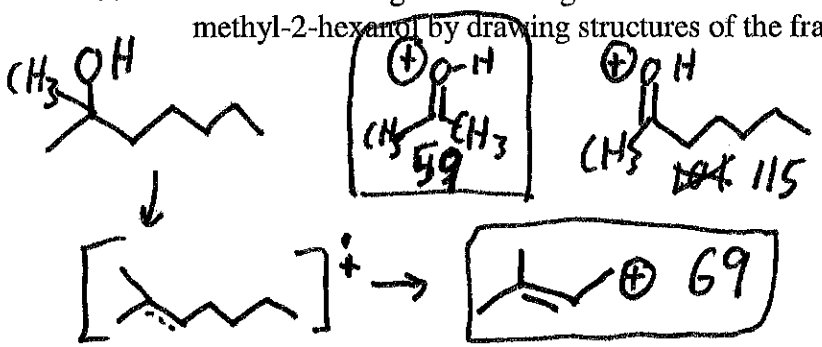
b) ^{1}H NMR Spectroscopy: aligns some nuclei to have an alpha spin & others a β spin.

8. A compound gave the following pattern in its mass spectrum. What characteristic element is contained in this compound? (2 points)

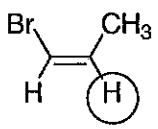


Cl

9. Account for fragments having a m/z value of 59 and 69 in the mass spectrum of 2-methyl-2-hexanol by drawing structures of the fragments. (4 points)



10. Predict the spin-spin splitting of the indicated proton below and state the value of each coupling constant. (5 points)



dq

d: J = 10 Hz

q: J = 7 Hz

11. In ^{1}H NMR spectroscopy, a peak located at 5.7 ppm would most likely correlate to which functional group. (2 points)

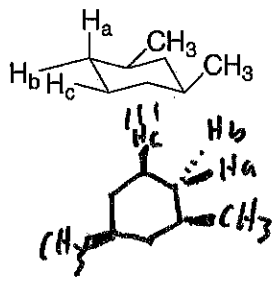
a) aldehyde b) aromatic ring c) ether (d) alkene e) carboxylic acid

12. Which of the following reasons best explains why aromatic protons have a larger chemical shift than protons one carbon removed from a halogen? (2 points)

a) An aromatic ring is more electron withdrawing than a halogen.
b) A halogen is more electron withdrawing than an aromatic ring.
c) Electron movement induces a magnetic field opposing the external field.
d) Electron movement induces a magnetic field reinforcing the external field.

13. (Circle the correct answers) Suppose a bare proton nucleus is in resonance when subjected to 60 MHz frequency in a particular magnetic field. When electrons are then added to the nucleus, resonance can be reestablished by either (increasing / decreasing) the applied frequency or (increasing / decreasing) the applied magnetic field. (4 points)

14. State the stereochemical relationship between the indicated protons below as homeotopic (same), enantiotopic, diastereotopic or none of the previous. (4 points)



H_a and H_b: diaster.

H_a and H_c: none of previous

15. What two factors related to carbon delayed the development of ^{13}C NMR spectroscopy? (4 points)

1) Low isotope abundance: ^1H: 100% vs. ^{13}C: 1%.

2) Low gyromagnetic ratio:

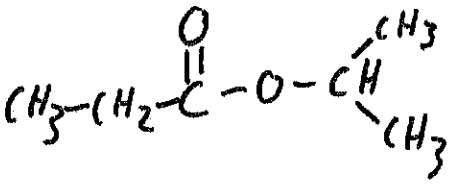
$\frac{1}{4}\gamma_{1H} = \gamma_{13C}$

II. Spectra interpretation and prediction

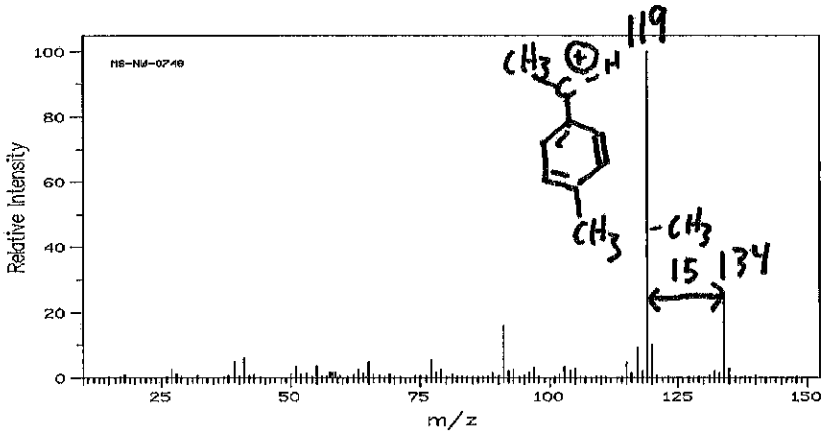
C=O 1° unsat

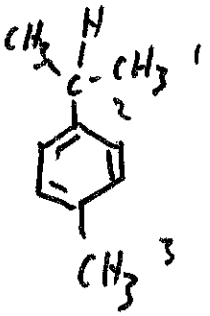
1. An unknown compound, $C_6H_{12}O_2$, gave the following **off-resonance** ^{13}C NMR information: (174 ppm, s; 67 ppm, d; 28 ppm, t; 22 ppm, q; 9 ppm, q). Provide a structure for this compound. (6 points)

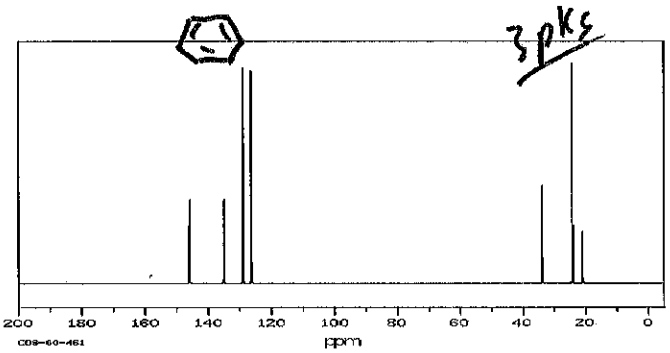
CH CH_2 CH_3 CH_3



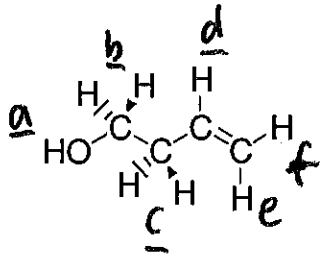
2. Provide a structure for compound **A** represented by the following mass spectrum and ^{13}C NMR spectrum. Justify your answer. (6 points)





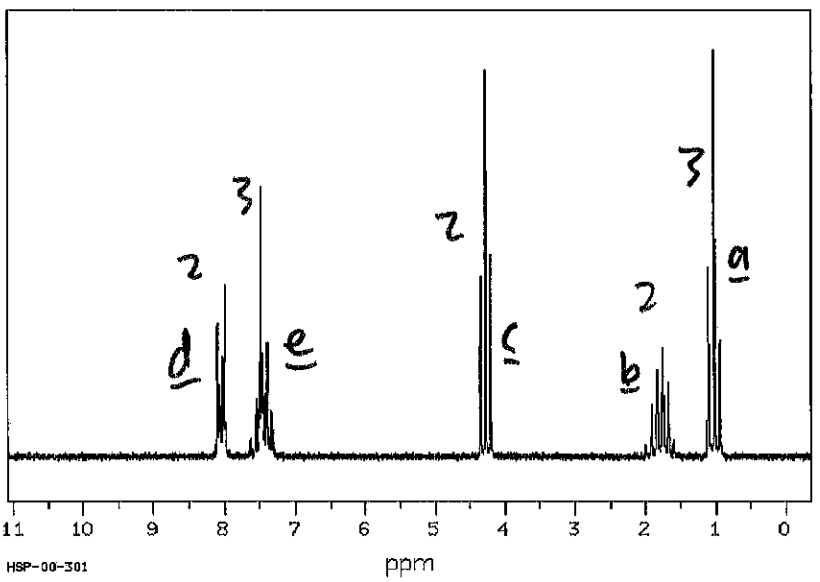


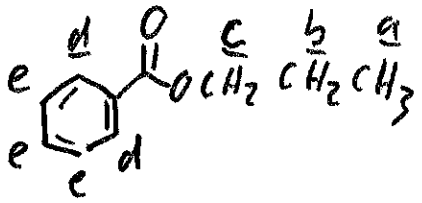
3. For the following compound, identify and label (a,b,c....) each different chemical environment. Predict the spin-spin splitting and chemical shift of each type of hydrogen. There may be fewer than 8 chemical environments. (10 points)



Type of hydrogen	a	b	c	d	e	f	g	h
Chem. Shift (ppm)	1-5	3.3	2.1	5.8	5.2	5.7		
Spin-spin splitting	s	t	dt	ddt	dd	dd		

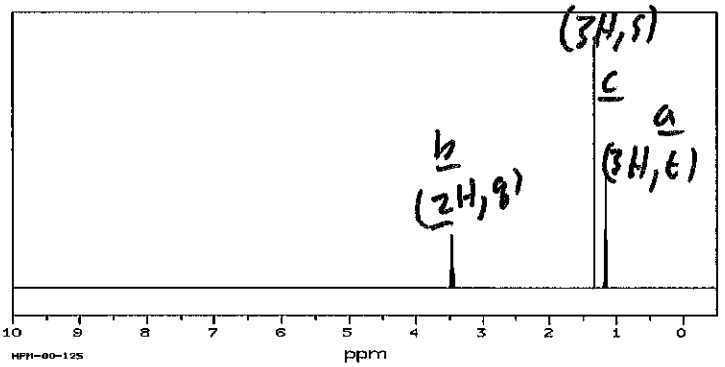
4. Identify the structure of compound **B** ($C_{10}H_{12}O_2$), which provided the following ^1H NMR spectrum shown below. Correlate each peak with each proton. (6 points)

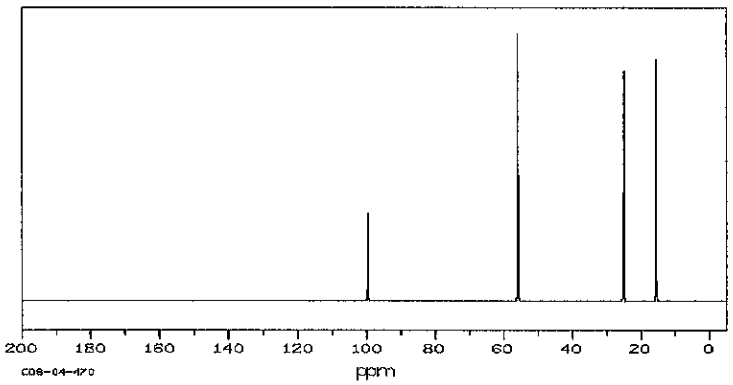


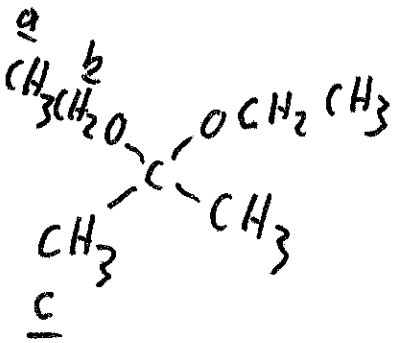


saturated

5. Use the following ^{1}H and ^{13}C NMR spectra to solve the structure of compound **C**, which has a molecular formula of $C_7H_{16}O_2$. Justify your answer by correlation of your structure with each spectrum. (6 points)



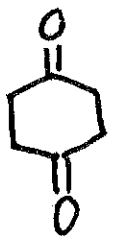




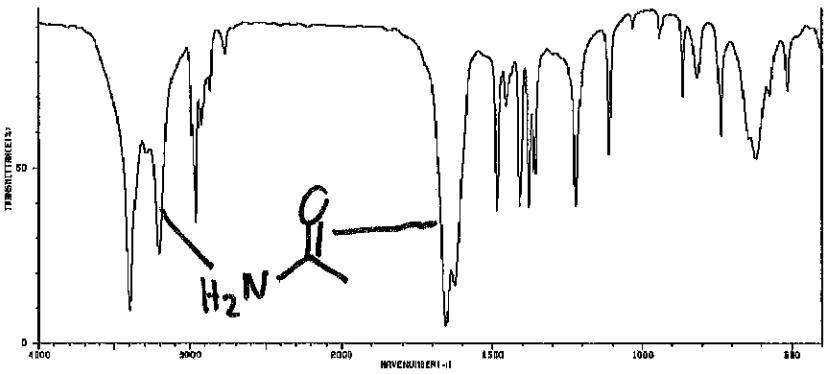
C=O

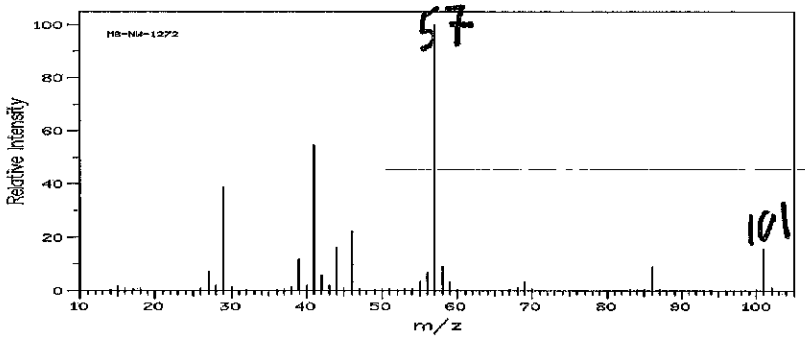
3° unsat.

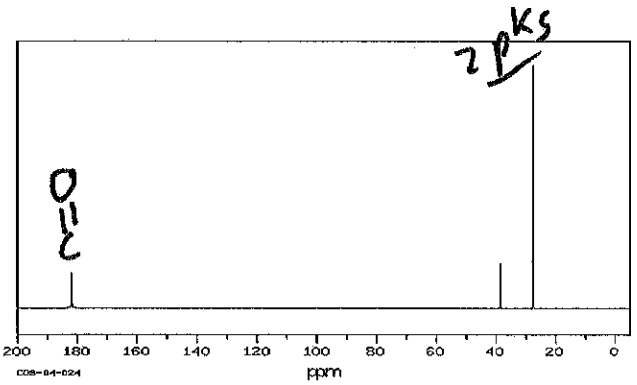
6. Given that compound **D** has a molecular formula of $C_6H_8O_2$, gave two peaks in its ^{13}C NMR spectrum (37 ppm and 208 ppm) but just one in its ^{1}H NMR spectrum (2.5 ppm), provide a structure for compound **D**. (5 points)

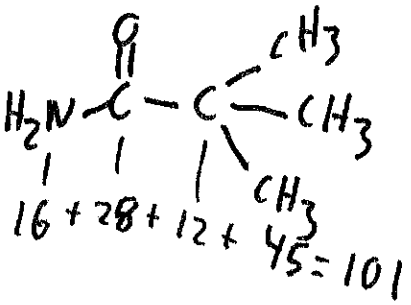


7. Use the IR, ^{1}H NMR and ^{13}C NMR spectra below to identify unknown compound E. Justify your answer by correlating the structure with each spectrum. (8 points)



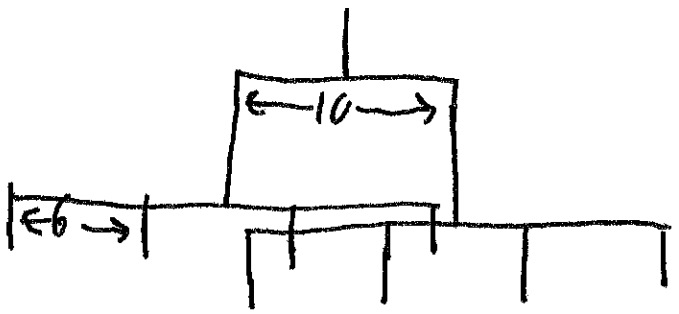


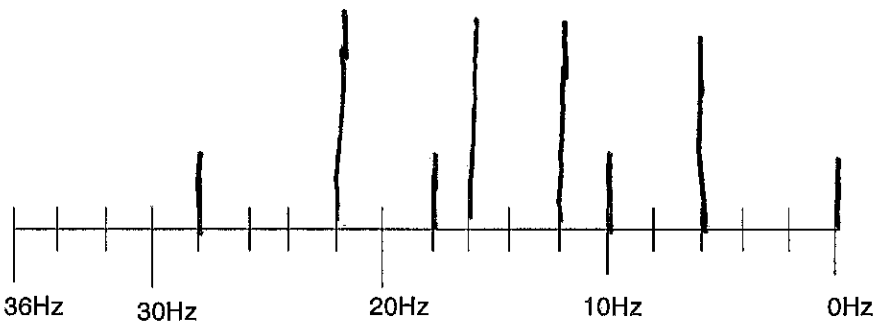




III. **Extra Credit** (5 points)

1. Using a splitting tree, predict the spin-spin splitting of a proton split into a doublet of quartets with coupling constants of J equal to 10 Hz and 6 Hz, respectively. Show peaks in the proper proportion and with the correct spacing. Begin the splitting pattern at 0 Hz. The grid below features 2 Hz / dash.





You received _____ points out of 100 points possible. To check your overall performance in lecture see http://vista.weber.edu