Fall 2320 E1

I. Theory

1. Which sequence correctly ranks the regions of the electromagnetic radiation spectrum in order of increasing energy? (3 points)

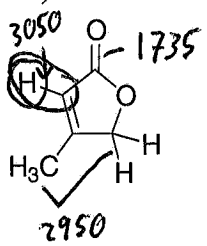
infrared low **1** ultraviolet high **2** visible **3**

a) 1<2<3 b) 2<3<1 c) 3<1<2 d) 3<2<1 e) 2<1<3 (f) 1<3<2

2. Circle all equations that are correct as written. (4 points)

a) $\lambda = \nu/c$ b) $\nu = h/\lambda$ (c) $E = hc/\lambda$ (d) $\Delta E = \gamma(h/2\pi)B_o$

3. Circle the bond in the following structure that has the highest IR absorption frequency value. (3 points)

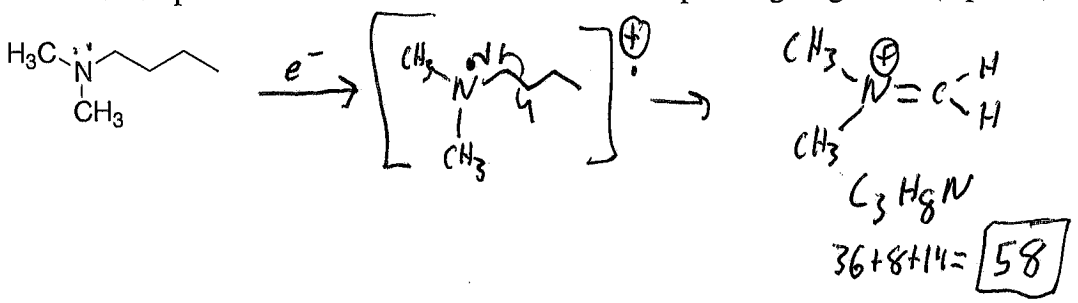


4. A(n) HETCOR NMR spectrum is a 2D NMR with a ^1H NMR scan along the y-axis and a ^{13}C NMR scan along the x-axis. (2 points)

5. Circle all species that may be detected by a mass spectrometer. (4 points)

a) H_2O (b) $[CH_3CH_3]^{\oplus\bullet}$ (c) $CH_3NH_3^{\oplus}$ d) $CH_3^{\bullet}$

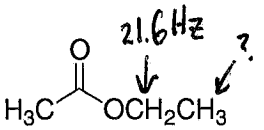
6. Predict the m/z value for the base peak of the following compound observed in its mass spectrum. Draw a structure for the corresponding fragment. (5 points)



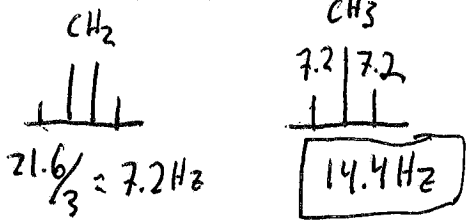
7. Low resolution mass spectrometry has a resolution of ____ amu. (2 points)

(a) 1 b) 0.1 c) 0.5 d) 0.01 e) 0.001

8. If the splitting pattern for the methylene group (CH_2) in ethyl acetate has a width of 21.6 Hz, what is the total width of the splitting pattern generated by the neighboring methyl group? (3 points)



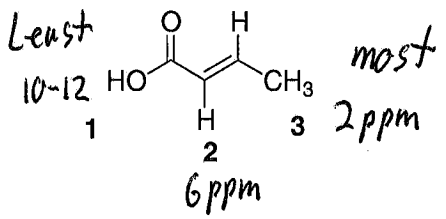
ethyl acetate



9. If a peak has a chemical shift of 3.5 ppm using a 300 MHz NMR, what is the value of this chemical shift in hertz? (3 points)

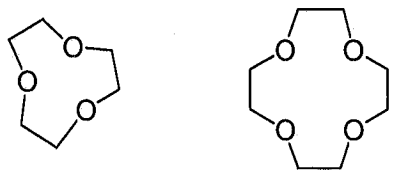
$\frac{3.5\text{ppm}}{1\text{ppm}} \times 300\text{Hz} = 1050\text{ Hz}$

10. Which sequence ranks the indicated protons in order of increasing amount of electron shielding in proton NMR spectroscopy? (3 points)



(a) 1<2<3 b) 2<3<1 c) 3<1<2 d) 3<2<1 e) 2<1<3 f) 1<3<2

11. Of the different analytical methods we have studied, which would be best suited for differentiating the following two structures? (2 points)



Mass Spec - Different MW

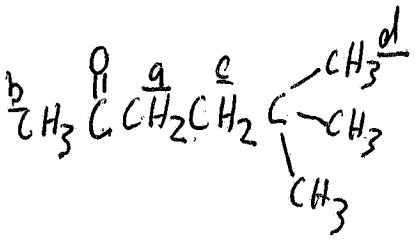
12. Which of the following spectroscopic methods provides the foundation for MRI examinations? (2 points)

a) IR b) UV / Vis (c) ^{1}H NMR d) ^{13}C NMR e) ^{31}P NMR f) x-ray

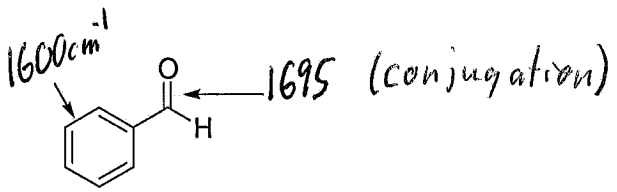
II. Spectra interpretation and prediction

1. Compound **A**, $C_8H_{16}O$, gave the following ^{1}H NMR spectrum: 2.4 ppm, triplet, 2H; 2.1 ppm, singlet, 3H; 1.5 ppm, triplet, 2H; 0.9 ppm, singlet, 9H. The compound also gave 6 peaks in its ^{13}C NMR spectrum. Propose a structure for compound **A**. (6 points)

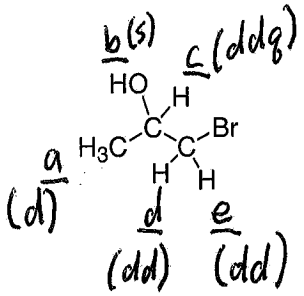
1° unsat.



2. Predict where stretching of the two indicated bonds would appear in an IR spectrum in wavenumbers. (4 points.)



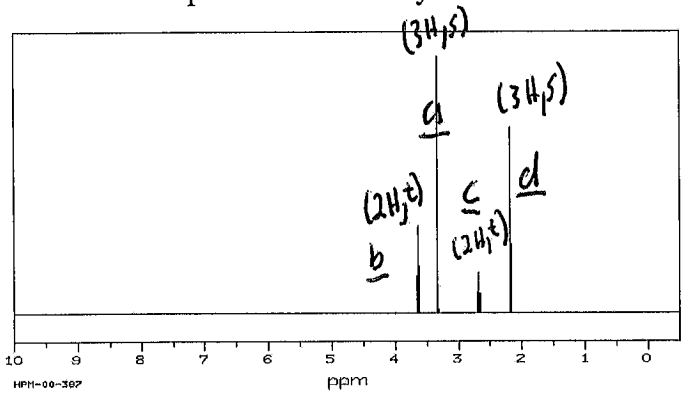
3. Alphabetically label each proton chemical environment, and then indicate the spin-spin splitting pattern of each proton environment in the structure below. (10 points)

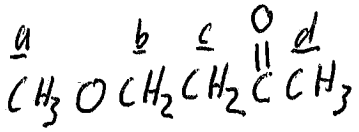


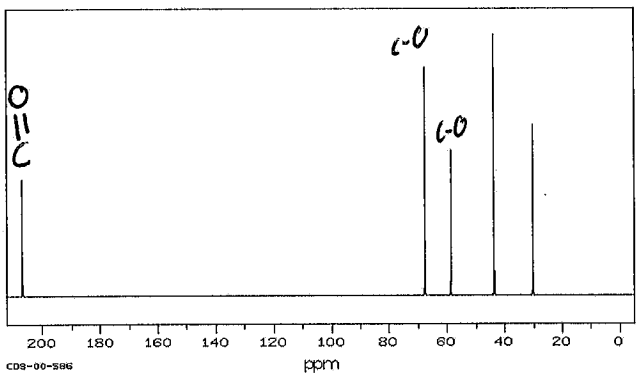
b (s) c (ddq) a (d) d (dd) e (dd)

1° unsat.

4. Identify compound **B**, $C_5H_{10}O_2$, from the following ^1H NMR and ^{13}C NMR spectra. Correlate your structure with each peak in both spectra. (10 points)

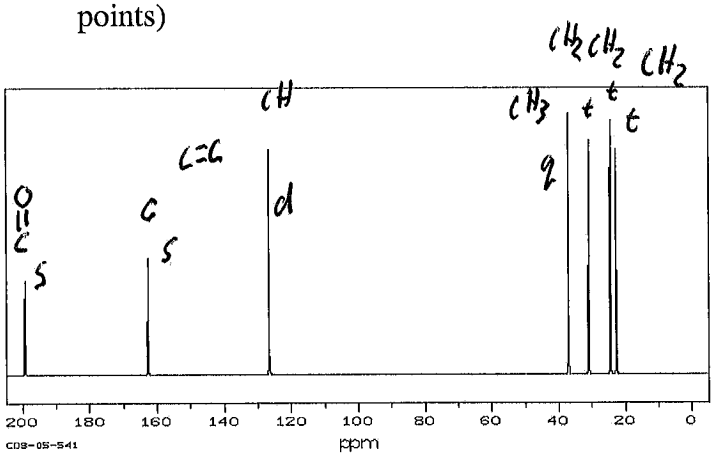


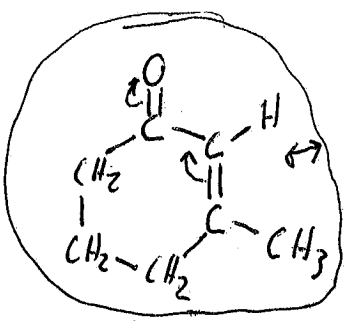


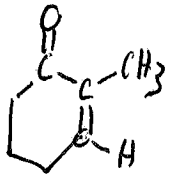


3° unsat.

5. Compound **C** has a molecular formula of $C_7H_{10}O$, and gave the following ^{13}C NMR with off-resonance coupling shown above each peak. Predict the structure and justify your answer through correlation with each peak in the spectrum. (8 points)

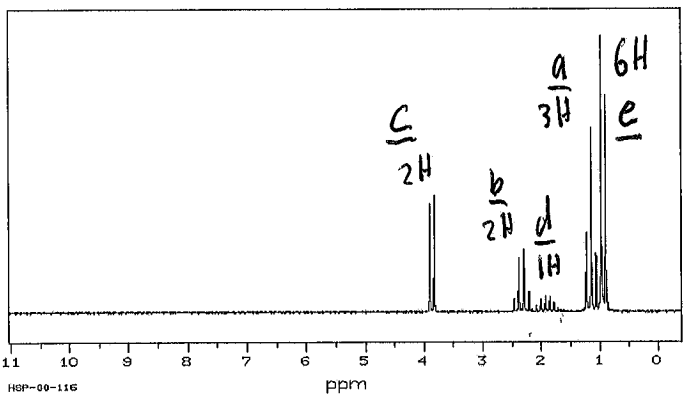


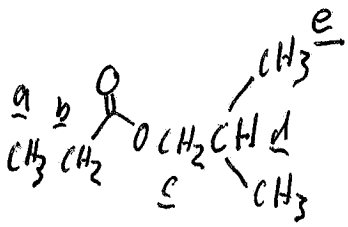




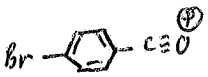
1° unsat.

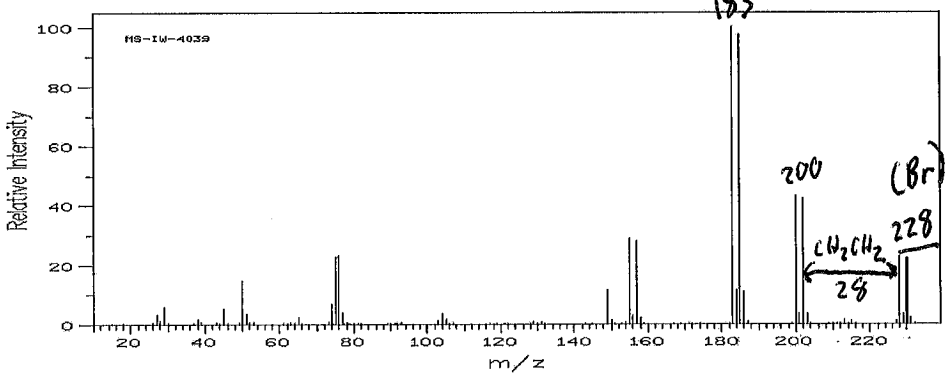
6. Compound **D**, $C_7H_{14}O_2$, gave the following 1H NMR spectrum. Provide a structure for compound **D** and justify your answer by correlation of the peaks with your structure. (8 points)





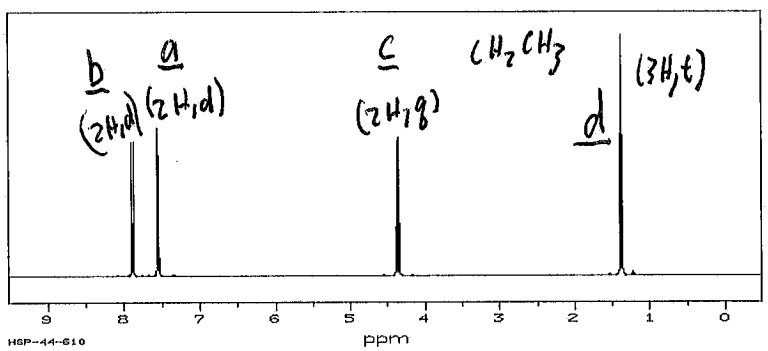
7. Provide a structure for compound **E**, given the following mass spectrum and ^1H NMR spectrum. Justify your answer through correlation of the structure with each spectra. (10 points)

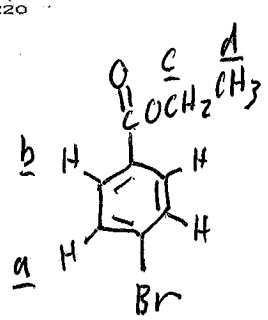




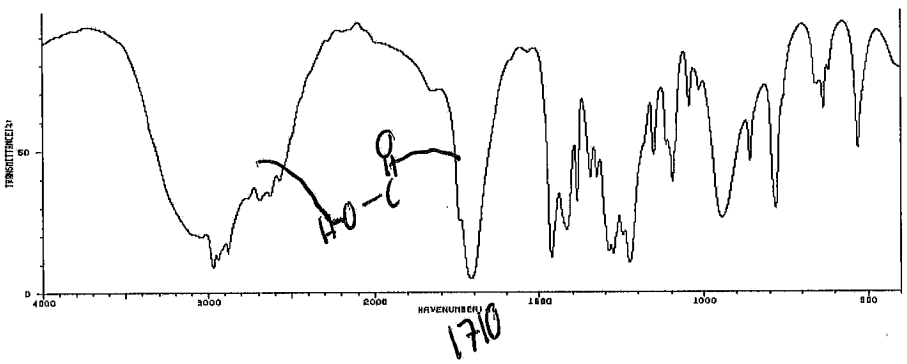
$C_9H_9O_2Br$

$108 + 9 + 32 + 79 = 228$





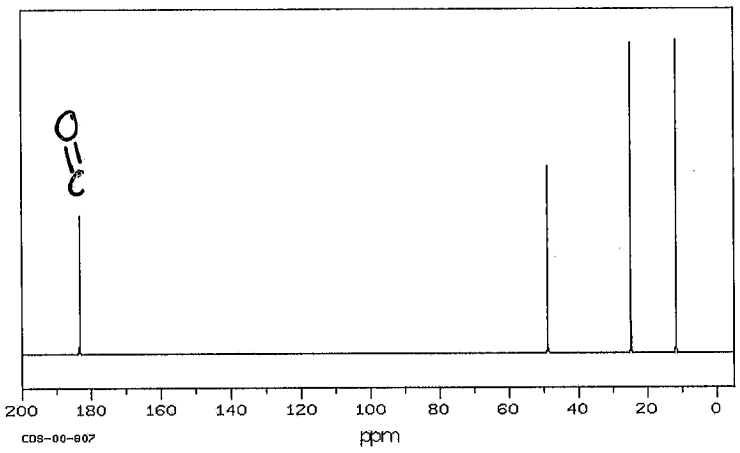
8. Identify compound **F**, having a molecular weight of 116, using the following IR and ^{13}C NMR spectra. Then **thoroughly** justify your answer by correlating your structure with the key peaks in each spectra. (8 points)

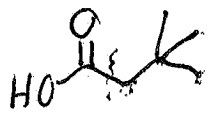


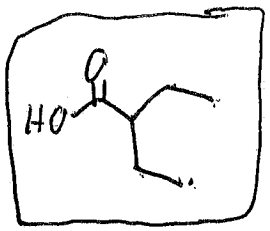
116
− 45 C-OH
71

5
12 | 71
60
11

C_5H_{11}

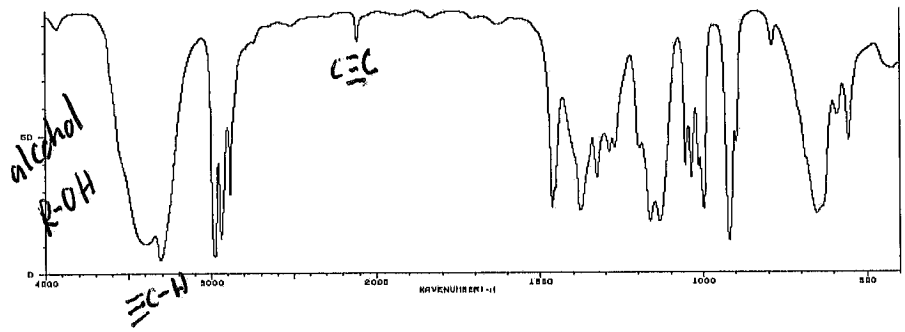






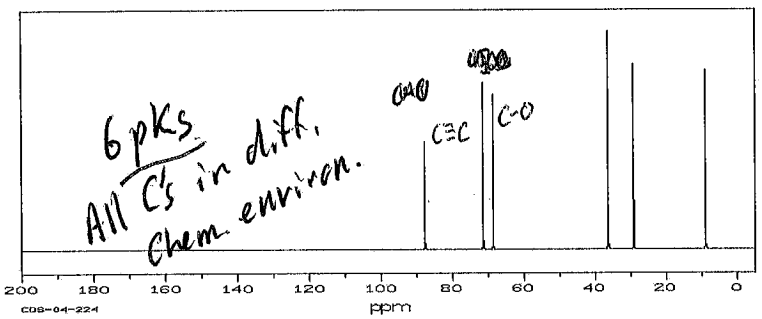
III. **Extra Credit** (5 points)

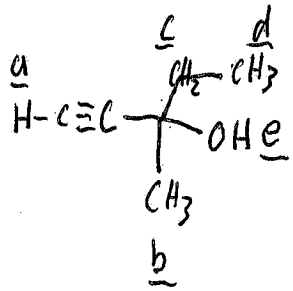
1. Identify compound **G** using the following spectra and given that the compound had a molecular ion peak of 98.

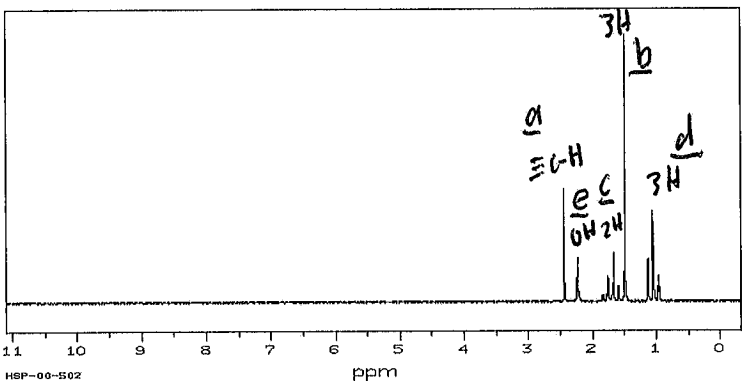


$C_6H_{10}O$

72+10+16







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