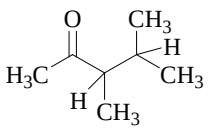
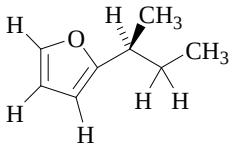
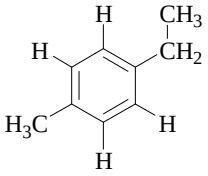
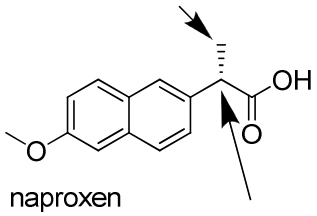
Chemistry 247 Hanson **SAMPLE EXAM 3** **(Oct. 25, 2010)**

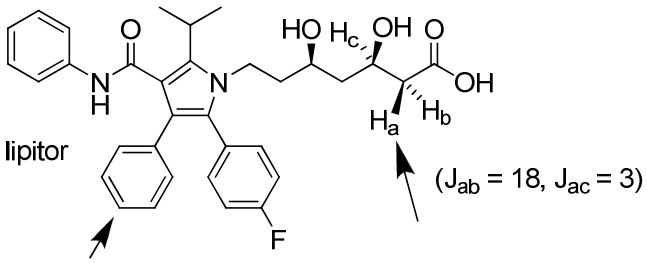
(18) 1. For each of the molecules below, circle sets of **NMR-equivalent hydrogen atoms** and indicate the number of different signals you expect in the ^{1}H and ^{13}C NMR spectra.

^{1}H:	_____ signals	_____ signals	_____ signals
^{13}C:	_____ signals	_____ signals	_____ signals

(12) 2. Draw the picture of the peak you expect to see in a ^{1}H NMR spectrum for each of the protons at the indicated positions.

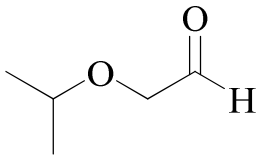




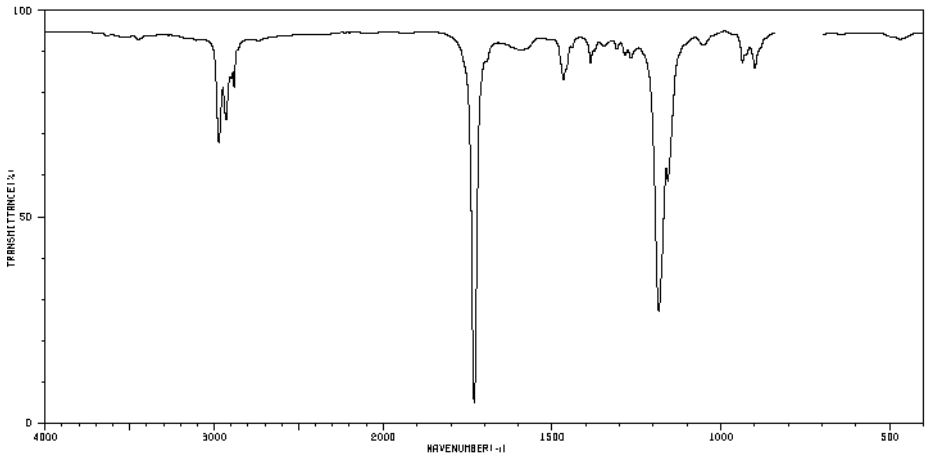
(20) 3. Explain briefly using just one or two sentences…

a. …the origin of the "chemical shift" -- Why protons in a molecule do not all absorb at the same frequency.
b. …why C-H single bonds absorb in the infrared at a much higher energy than C-C single bonds.
c. …what the "finger print" region is, and why it is called that.
d. …the terms "base peak" and "molecular ion"
e. …how it is possible to have two hydrogen atoms on adjacent carbon atoms that appear as singlets in the NMR spectrum.

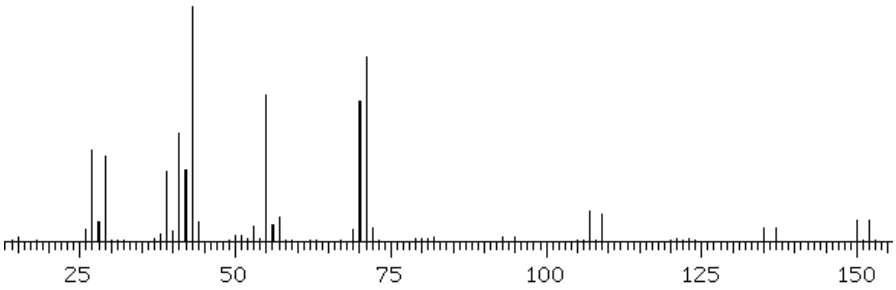
(12) 4. Predict the ^{1}H NMR spectrum of the compound shown here. Show appropriate chemical shifts, integrations, and splitting patterns.



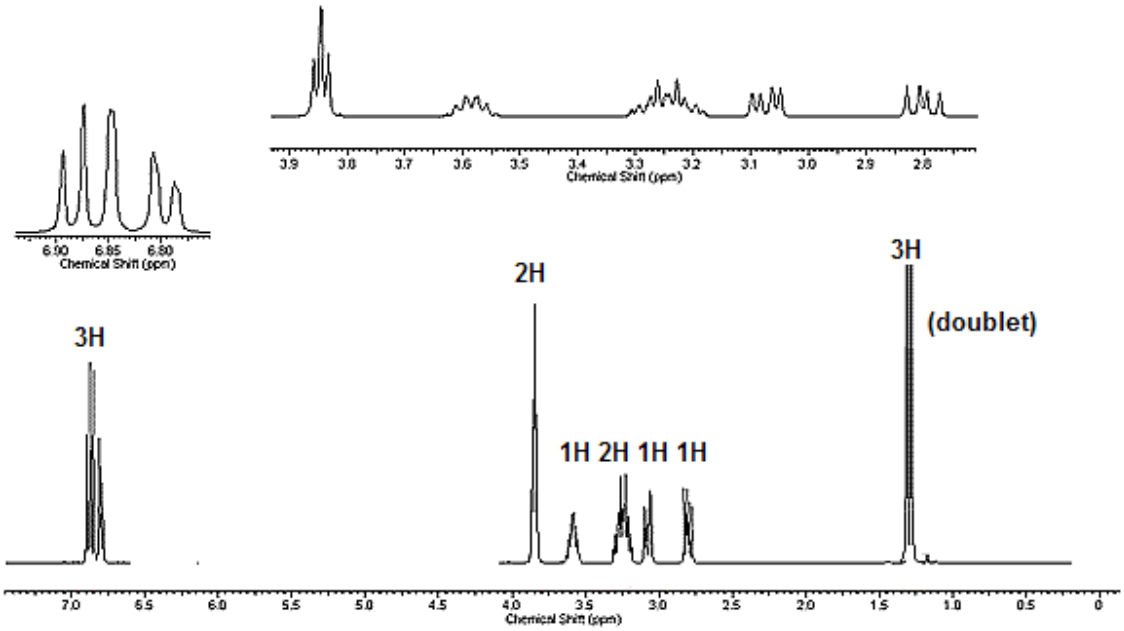
(6) 5. Find three clues about a structure that can be deduced from the IR spectrum shown on the right, with formula C_4H_8O. [HINT: What is NOT present can be as important as what IS present.]



(6) 6. Find three clues about a structure that can be deduced from the mass spectrum shown below. [HINT: What is NOT present can be as important as what IS present.]

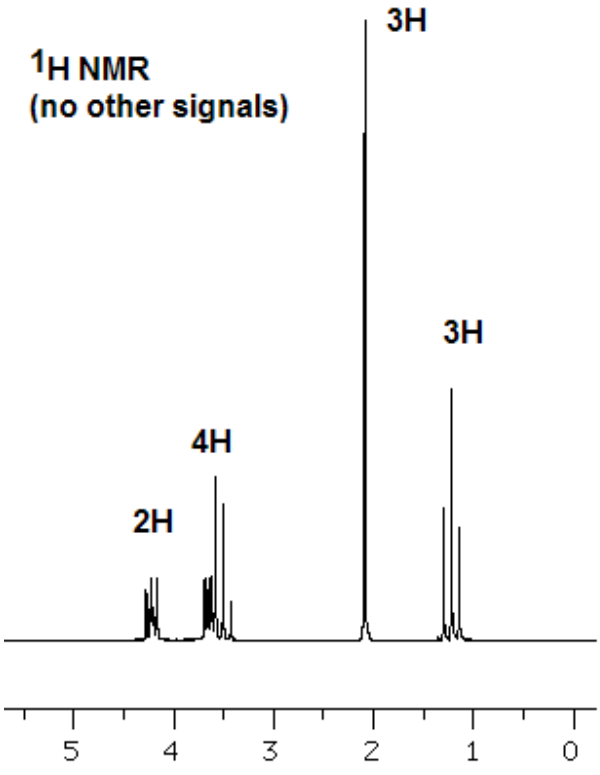


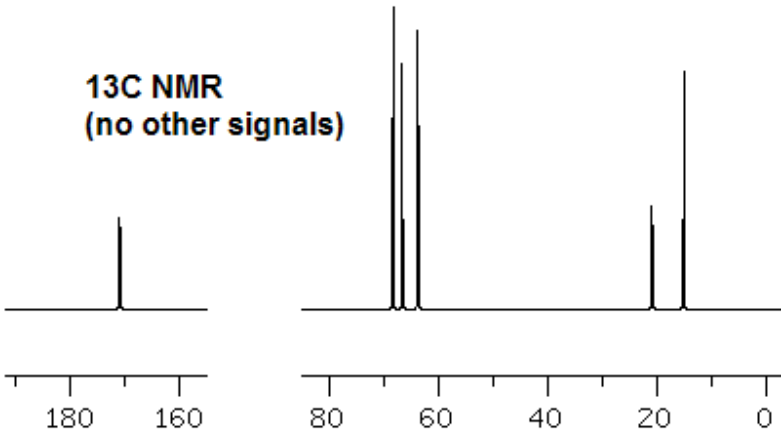
(6) 7. The spectrum below is of a compound recently found in France as part of a drug bust. Given the ^{1}H NMR spectrum below, identify **just three aspects** of this illegal substance. In this case, tell me specifically what you think IS present in the molecule, not what is not present.



ref: http://www.justice.gov/dea/programs/forensicsci/microgram/journal_v3_num34/journal_v3_num34_pg7.html

(25) 8. Determine the structure of the compound with molecular formula $C_6H_{12}O_3$ (MW 132) having the spectral data shown on the next page. Be sure to make a clear argument for the structure you have decided upon that involves ALL four spectra. (You can do this just by annotating the spectra.)





NOTE: For our purposes here, you may consider the two relatively messy signals at δ 4.2 and 3.6 to be triplets. One of those signals also overlaps with something else at δ 3.5.

(For 5 bonus points, after you get your structure, explain using a Newman projection why the signal at δ 4.2 would NOT be a simple triplet.)