Problem Set 7

Name_____
SID_____

1) A photon of electromagnetic radiation contains 7.98 x 10^5 kJ/mol of energy

A) (2 pts) What is the frequency (in Hz) of the radiation for this photon?

B) (2 pts) What is the wavelength (in meters) for this radiation?

C) (2 pts) What is the wavelength in Angstroms?

D) (2 pts) With what region of the electromagnetic spectrum does this correspond?

E) (2 pts) How does this wavelength correspond to the average C-C single bond length (look back to chapter 1 for this)?

One of the ways matter can interact with molecules is by reflecting it (actually, diffracting it). Radiation at this particular wavelength does not get absorbed, but is reflected by individual atoms. It is not affected by the electrons in chemical bonds. For this reason, we can use radiation in this range of wavelength to determine the position of atoms in a molecule...we can determine the actual 3-dimensional structure of molecules. While we won't discuss this particular application in Organic I or II, you can see why this would be a useful technique for organic chemists.

2) Consider a photon of electromagnetic radiation with a wavelength of 5.9×10^{-6} m.

A) (3 pts) What is the energy (in kJ) associated with this wavelength?

B) (3 pts) What is the wave number (reciprocal centimeters, cm^{-1}) associated with this wavelength?

C) (3 pts) What functional group absorbs at this energy?

D) (1 pt) Is this a stretching or bending mode of vibration?

3) (2 pts each) With which functional group does each of the following IR absorption frequencies correspond? (Intensity of absorption is in parentheses.)

A) 2200 - 2250 cm^{-1} (medium)

B) 1600 - 1680 cm^{-1} (weak to medium)

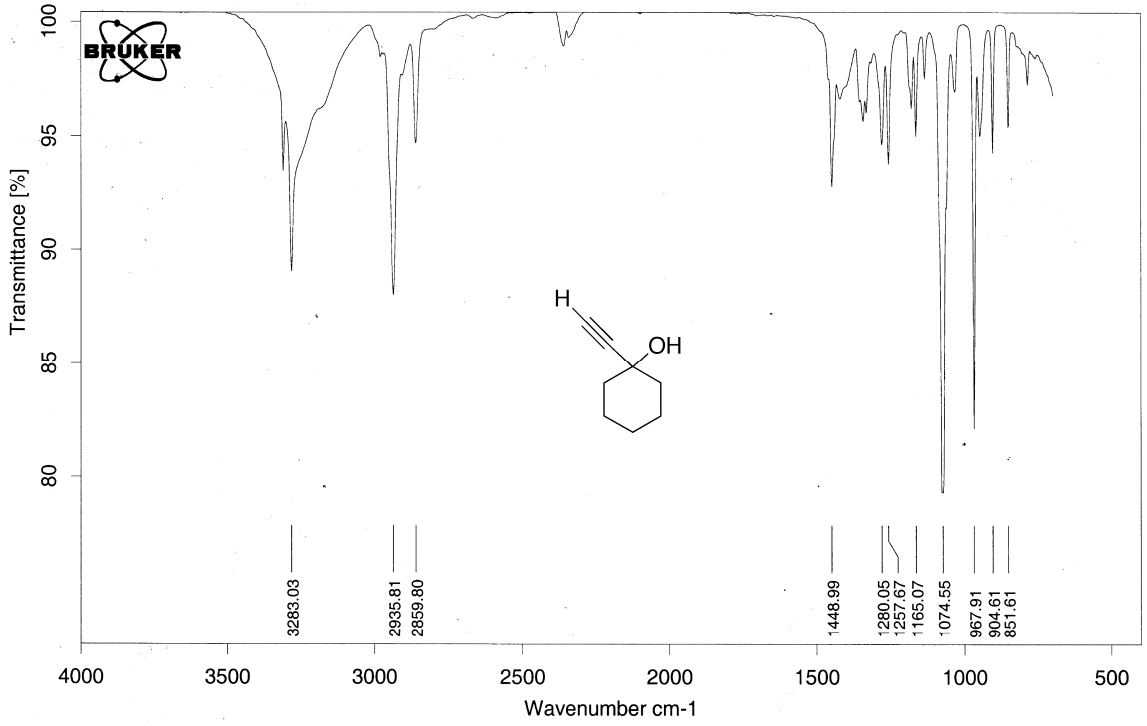
C) 1000 - 1100 cm^{-1} (strong)

D) 2850 - 3000 cm^{-1} (weak to medium)

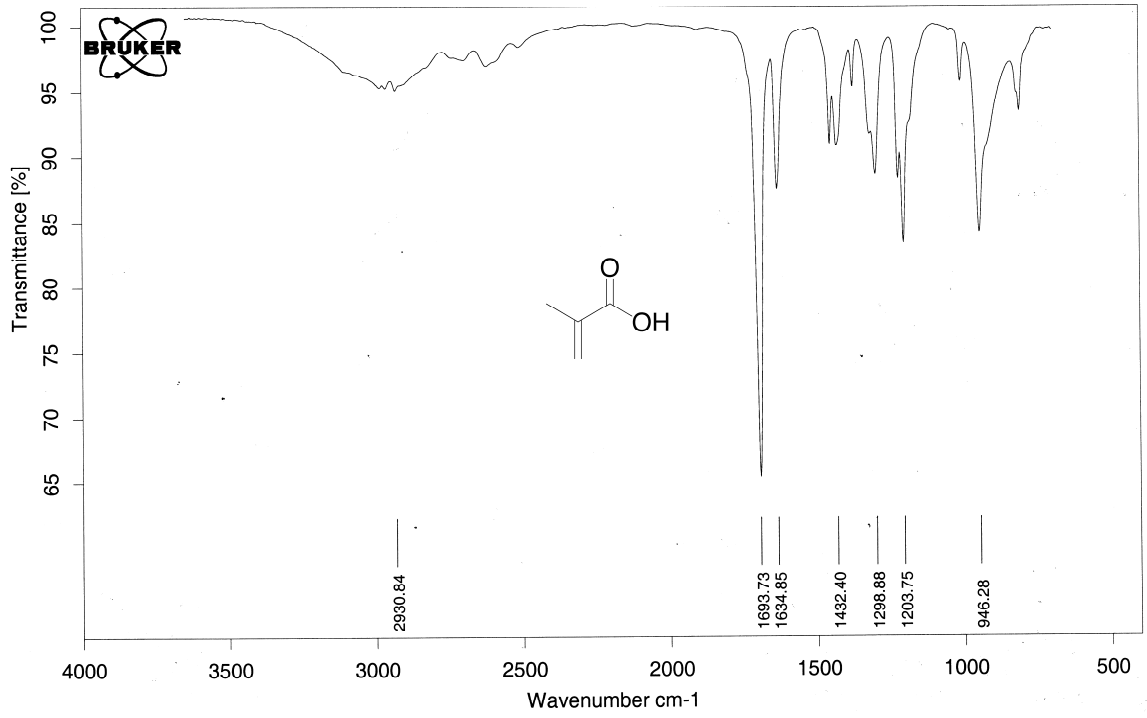
E) 1630 - 1680 cm^{-1} (strong)

4) (5 pts each) For each of the following spectra, assign the absorptions to the functional groups that causes them.

A) 1-ethynyl-1-cyclohexanol

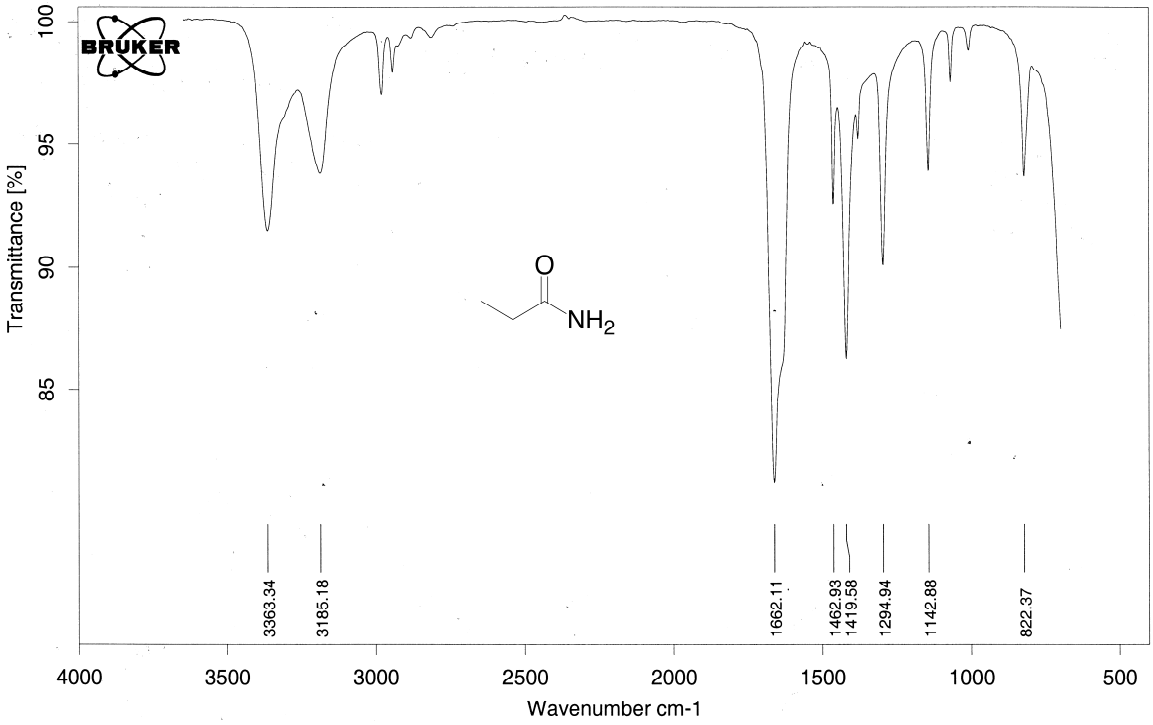


B) methacrylic acid

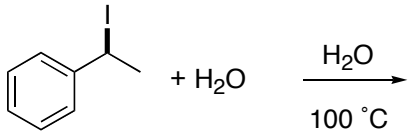


4) continued....

C) proprionamide



5) Consider the following reaction conditions:

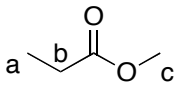


A) (4 pts) What do you expect to be the major product?

B) (2 pts) Will the product be optically active, racemic, or achiral?

C) (4 pts) In the IR spectra, what would be the major difference between the spectrum of the starting material and the spectrum of the product?

6) Consider the following molecule:



A) (2 pts) How many signals would you expect to see in the ^{1}H NMR spectrum?

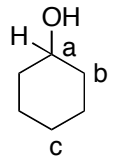
B) (2 pts) Into how many lines would the signal arising from the hydrogens on carbon *a* be split?

C) (2 pts) Into how many lines would the signal arising from the hydrogens on carbon *b* be split?

D) (2 pts) Into how many lines would the signal arising from the hydrogens on carbon *c* be split?

E) (2 pts) Which of the signals would you expect to be the most deshielded (at the highest ppm)?

7) Consider the following molecule:



A) (2 pts) How many signals would you expect to see in the ^{1}H NMR spectrum?

B) (2 pts) Into how many lines would the signal arising from the hydrogen on carbon *a* be split?

C) (2 pts) Into how many lines would the signal arising from the hydrogens on carbon *b* be split?

D) (2 pts) Into how many lines would the signal arising from the hydrogens on carbon *c* be split?

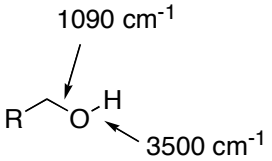
E) (2 pts) Which of the signals would you expect to be the most deshielded (at the highest ppm)?

8) A molecule with the molecular formula $C_5H_{10}O$ has the following IR and NMR spectral data: IR (neat): 2872 (m), 2903, 1708 (s), 1450 (w), 1396 (w) cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 2.42 (q, 4 H), 1.07 (t, 6 H).

To read this data, the following are general rules:
IR: values are listed from high wave number to low wave number. Letters in parentheses correspond to the intensity of the absorption: w = weak, m = medium, and s = strong.
NMR: Field strength and solvent are listed first. Chemical shifts are listed from high ppm to low ppm. The symbol δ means parts per million (ppm). Within parentheses following each chemical shift are two values. First is the splitting pattern: s = singlet, d = doublet, t = triplet, and q = quartet. Last is the integration: "*n* H" = *n* hydrogens generating the signal.

A) (5 pts) Propose a structure for the molecule.

B) (10 pts) Correlate the spectral data to the structural feature that produced the absorption. For example, the structure below shows a generic alcohol with the IR stretch assigned. You can do something similar for the NMR data.



Extra Credit: (10 pts) A molecule with molecular formula $C_9H_8O_2$ decolorizes bromine and has the following spectral data:

IR (neat) 3056 (b), 2966 (m), 2927 (w), 2855 (w), 1680 (s), 1620 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 11.00 (bs, 1 H), 7.81 (d, 16.1 Hz, 1 H), 7.56 - 7.40 (m, 5 H), 6.47 (d, 16.1 Hz, 1 H); ^{13}C NMR (25 MHz) δ 172.76, 147.11, 134.11, 130.74, 128.40, 117.44.

What is the structure of the molecule? Hint: Pay particular attention to the problem solving section in Chapter 13.15. In addition to the general rules listed in problem 8 for reading the spectral data, keep these thoughts in mind:

IR: b = broad. NMR: ^1H NMR data can have ranges of ppm for a signal, not just a single value for chemical shift. The information in parentheses can have three values. When that happens, the middle value is the coupling constant for the splitting. b = broad, and can "modify" any of the normal splitting patterns. "bs" is a broad singlet. m = multiplet (more than 4 lines for the signal). ^{13}C NMR data is simply a list of chemical shifts. All chemical shifts are relative to TMS.