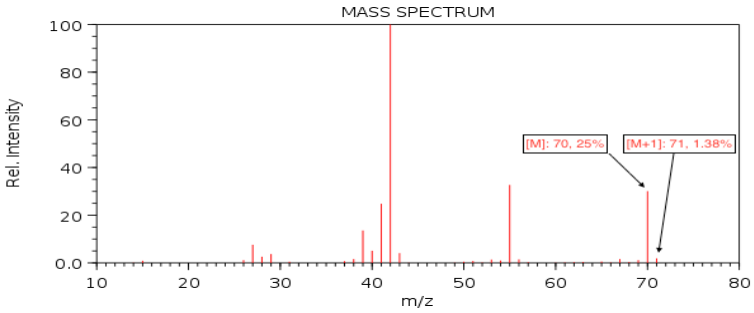
Homework 5
Organic Chemistry I (CHM 221/223) • Prof. Chad Landrie

Score (4 pts)		Lectures	10, 11	Name	

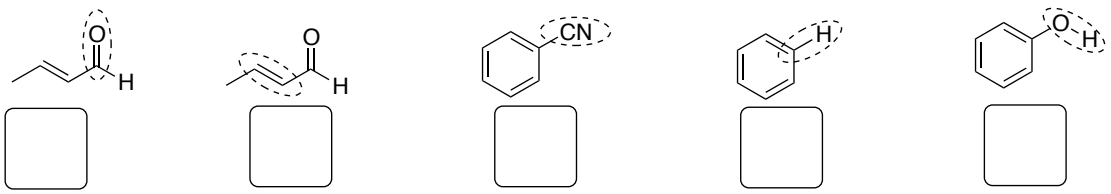
1. The mass spectrum for an unknown hydrocarbon showed that the [M] and [M+1] peaks had intensities of 25% and 1.38%, respectively. If the relative abundance of ^{13}C is 1.1%, how many carbon atoms are in the unknown hydrocarbon? Show all work. No credit for guessing. Wrong work = no credit.



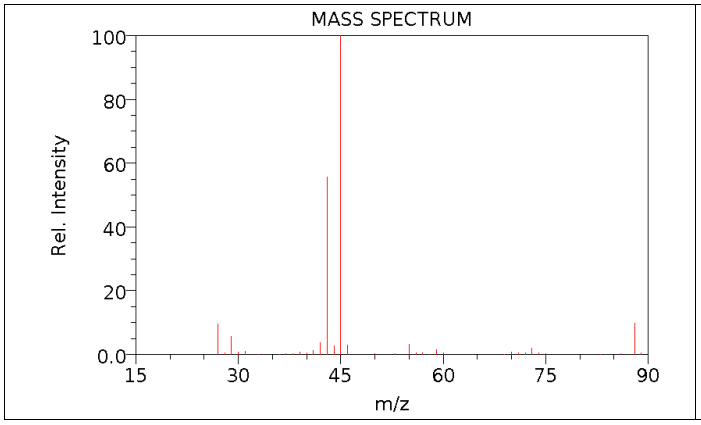
2. Predict the ratio of peak heights in an isotopic cluster for the $[M]^+$, $[M+2]^+$ and $[M+4]^+$ signals in a compound with a molecular formula of C_2H_4BrCl. Show all work.

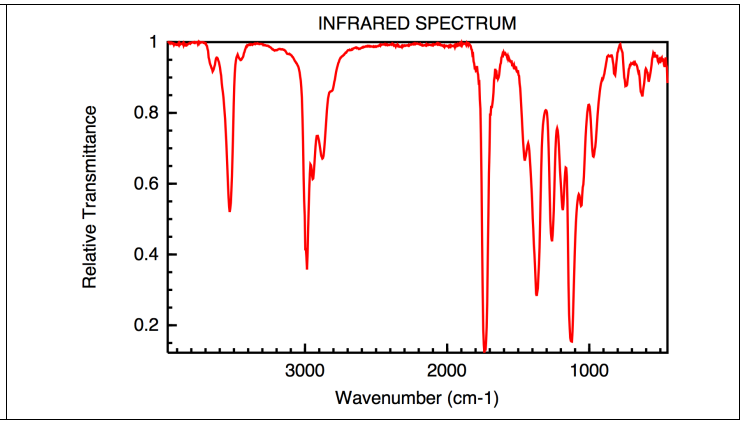
3. Conjugated (adjacent π-bonds) carbonyl compounds have a lower stretching frequency than non-conjugated carbonyl bonds. First, draw an example of a conjugated ketone and a non-conjugated ketone. Second, state what two factors affect the IR stretching frequency of a covalent bond. Third, explain why the conjugated ketone has a lower stretching frequency. You will need to draw additional diagrams to illustrate your answer.

4. Rank each circled bond in order of increasing wavenumber ("frequency") for the stretching motion in infrared spectroscopy (1 = lowest wavenumber; 5 = highest wavenumber).



5. The CSI lab found traces of an unknown substance at the scene of a crime. It was found to be soluble in CH_2Cl_2, but insoluble in either aqueous acid or aqueous base. Elemental analysis of the substance was found to contain: 54.53% C, 9.15% H, and 36.32% O by mass. Infrared and mass spectra were also acquired. Unfortunately, the compound did not match any substances in their library so they had to call in real chemists (you!) to deduce the structure.





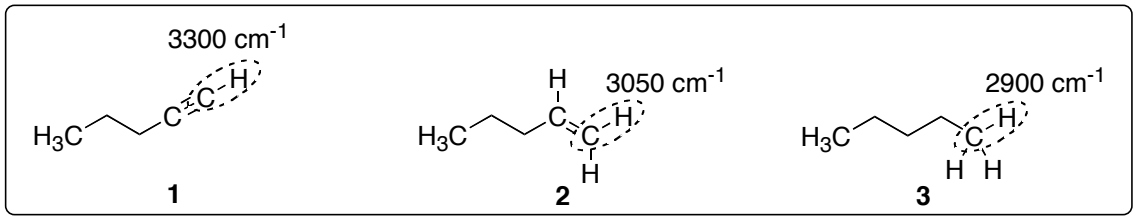
a. First, determine the molecular formula from the elemental analysis and MS data. Show all work.

b. Second, determine the index of hydrogen deficiency (the number of double bonds and/or rings) from the molecular formula.

c. Third, list the functional groups indicated by the IR spectrum and then draw your proposed structure below.

d. Based on your structure above, draw two cation (or radical cation) fragments that could account for the m/z signals at 43 and 45.

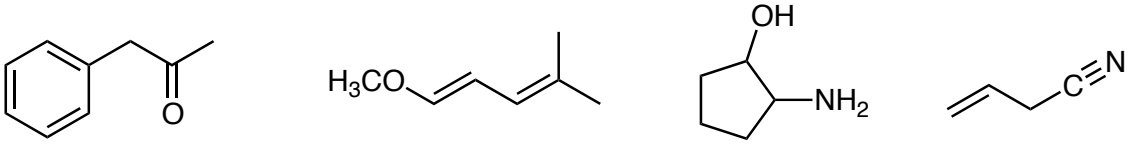
6. Briefly explain the variation in IR stretching frequency for the C-H bonds in the molecules below. Include a discussion of hybridization, the orbital overlaps that makeup the C–H σ-bond, bond strength and Hooke's law. You may also draw diagrams (e.g., valence bond orbitals) if they will aid in your discussion.



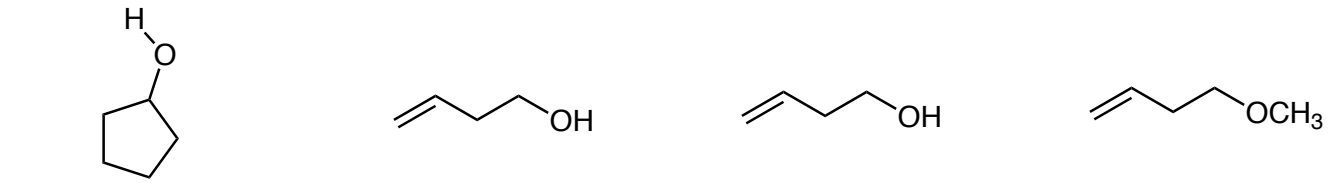
7. List the two factors that effect the <u>intensity</u> of an IR stretching band. Be specific. "Bond type" is too general.

8. List the two factors that effect the <u>frequency</u> of an IR stretching band. Be specific. "Bond type" is too general.

9. Circle the molecule(s) below that you would expect to exhibit a very intense and sharp band around 1700 cm^{-1}. Circle all that apply.



10. First, circle the sample below that you would expect to exhibit an intense and sharp band around 3200 cm^{-1}. Second, draw a square aound the sample that you would expect to exhibit an moderately intense and broad band around 3200 cm^{-1}.



sample phase = gas
concentration = N/A

sample phase = solution
concentration = 2.0 M

sample phase = solution
concentration = 0.2 M

sample phase = solution
concentration = 0.5 M

11. Write the letter corresponding to each molecule in the circle within its respective infrared spectrum. Each letter is only used once.