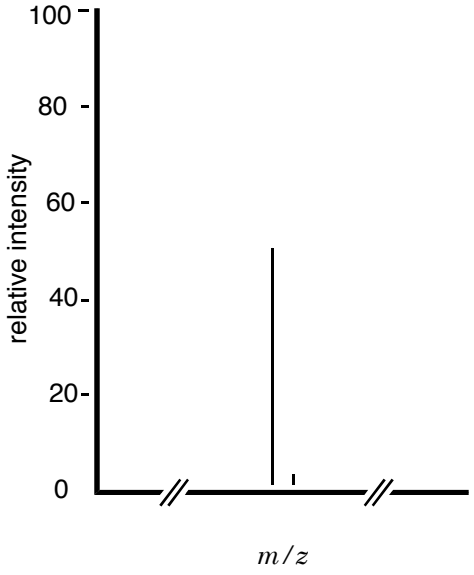
Name _____ Test 3 (4/15)
CHEM 0203 (Organic II) Spring 2009

1. A mass spectrogram contains a peak arising from a fragmentation of the molecular ion that has an m/z ratio of 86.07. Its relative intensity is 50%. At an m/z of 87.07, there is a smaller peak with a relative intensity of 2.7%.



// Indicates a break in the spectrogram. Only the peaks of interest are shown.

a. (8 pts.) Explain the relationship between the peak at 86.07 and the peak at 87.07.

b. (4 pts.) Determine the number of C atoms in the fragment that gives rise to the peak at 86.07.

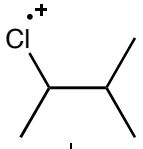
c. (2 pts.) Determine the number of C atoms in the fragment that gives rise to the peak at 87.07.

1. _____
2. _____
3. _____
4. _____
5. _____
6. _____
7. _____
8. _____
9. _____

2. Alkyl halides can undergo homolytic cleavage reactions.

a. (8 pts.) Determine the fragments that can form during the homolytic cleavage reactions that the alkyl halide drawn below can undergo.

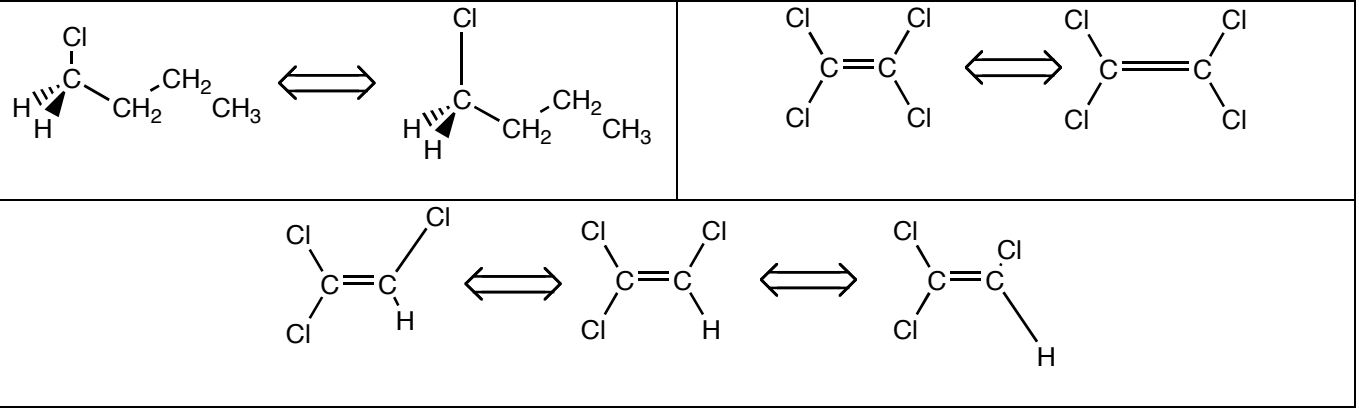
b. (6 pts.) Determine the mass to charge ratio for the fragments that will be detected by the mass spectrometer.



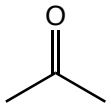
3. Molecules vibrate in a great many way, but only certain vibrational modes can absorb infrared light.

a. (3 pts.) What must the vibrational mode do in order to absorb infrared light?

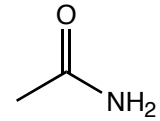
b. (3 pts. each) Which of the following vibartional modes would absorb infrared light?



4. (8 pts.) A typical carbonyl, like the one found on acetone, has a stretching frequency near 1715 cm^{-1}. Amides, on the other hand, have lower stretching frequencies. Explain why the stretching frequency of the amide is lower. In your explanation, remember to consider how the strength of a bond affects its stretching frequency. The structure of acetone and an amide are provided for your reference.

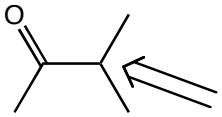


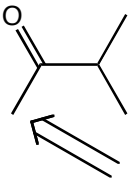
acetone

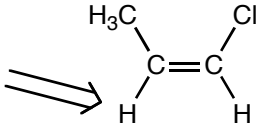


methylamide

5. (12 pts.) Determine the multiplicity of peak that results from the indicated proton(s).

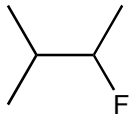
a. 

b. 

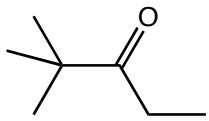
c. 

6. (10 pts.) Determine the relative positions of the protons on the following molecules. Label the protons alphabetically starting with the protons that resonate at the highest frequency. Chemically equivalent protons should be labeled with the same letter.

a.



b.



7. (10 pts.) For the molecules in question 6, determine the relative areas (the integrations) for each peak that you expect to see. Use the same labeling scheme here as you did in question 6.

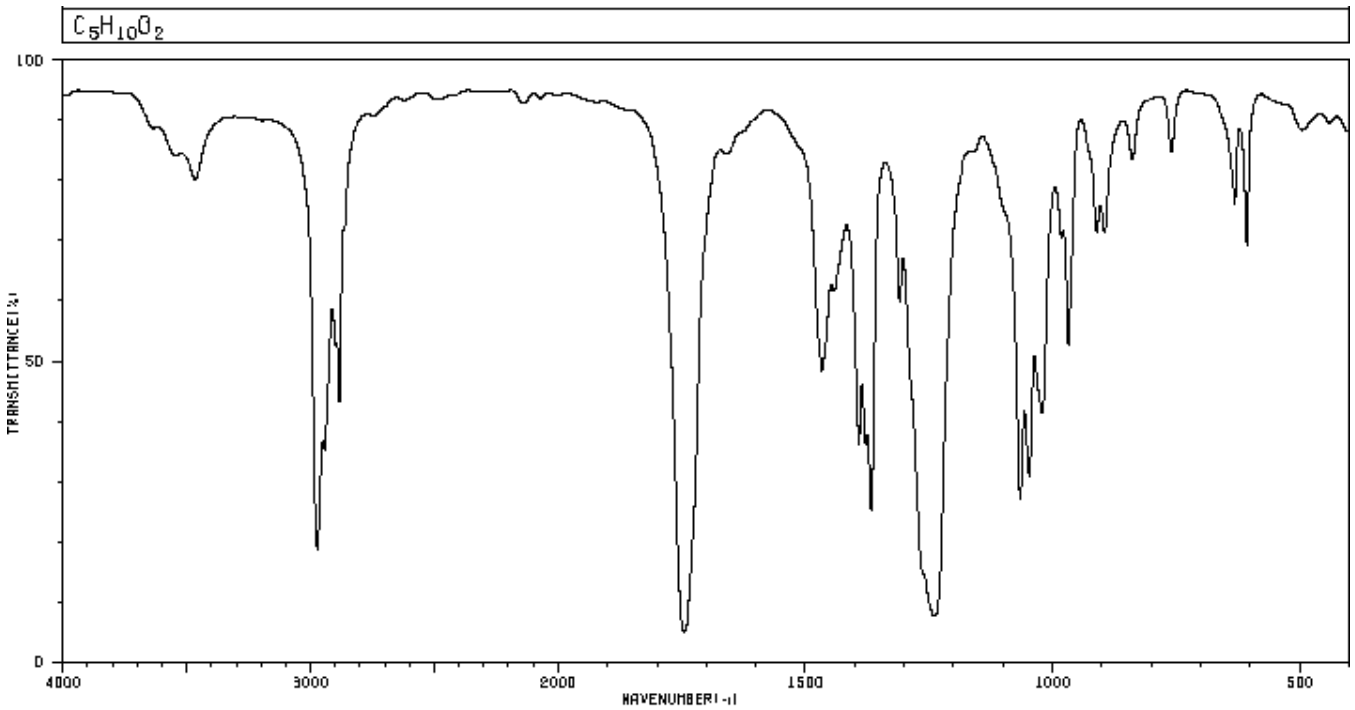
a.

b.

8. On the following page, IR data and NMR data are provided for a molecule with the formula $C_5H_{10}O_2$.

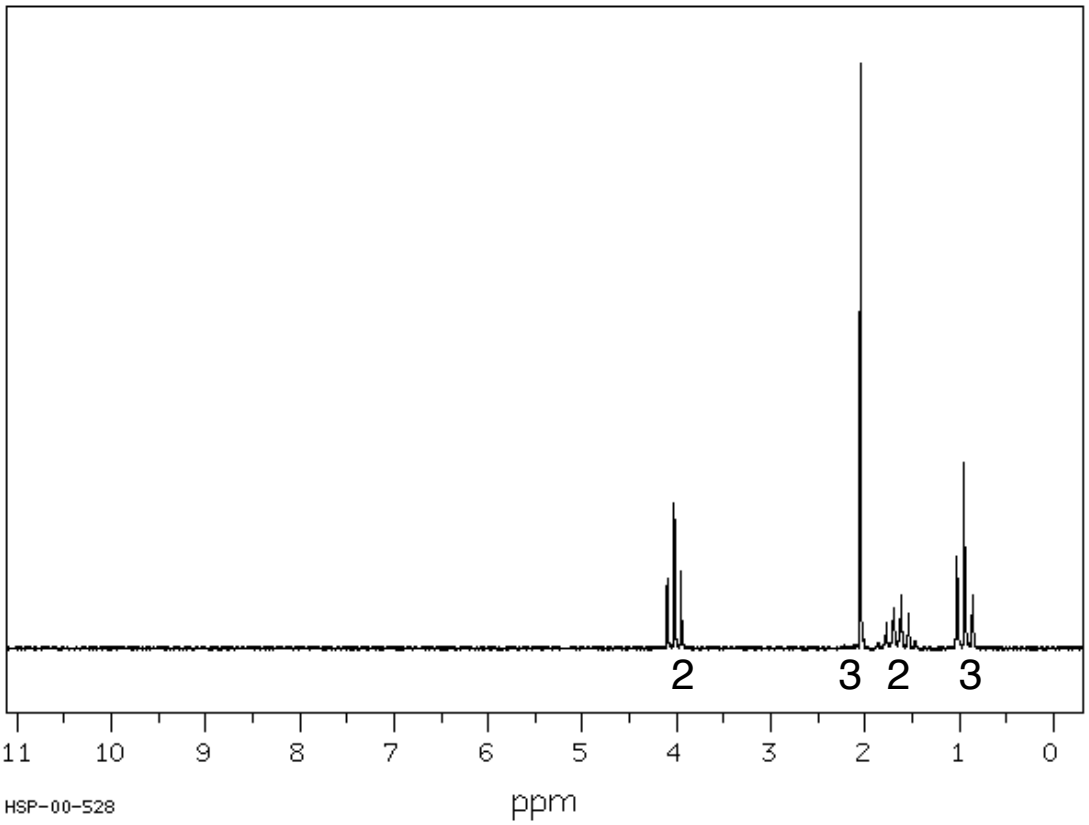
a. (8 pts.) Determine the functional groups on the molecule, and assign the peaks in the IR spectrum to those functional groups (be specific).

b. (8 pts.) Determine the structure of the molecule and label the peaks in the NMR spectrum that correspond to the protons on the molecule (label the molecule with letters and label the corresponding peaks with the same letters).

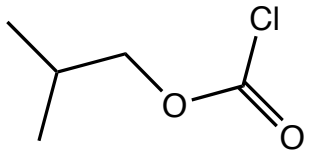


3466	77	1392	34	1021	39	760	81
2973	18	1378	34	982	68	632	72
2942	34	1367	24	968	50	607	66
2898	60	1309	67	911	68	496	84
2883	41	1238	7	895	68	440	86
1745	4	1065	26	845	84		
1467	46	1047	29	839	81		

ppm	height
4.1	120
4.025	250
3.95	134
2.05	1000
1.771	45
1.698	69
1.693	68
1.624	51
1.614	92
1.537	59
1.023	157
0.945	316
0.937	174



9. The proton and carbon NMR for a molecule with the formula $C_5H_9O_2Cl$ are provided below.



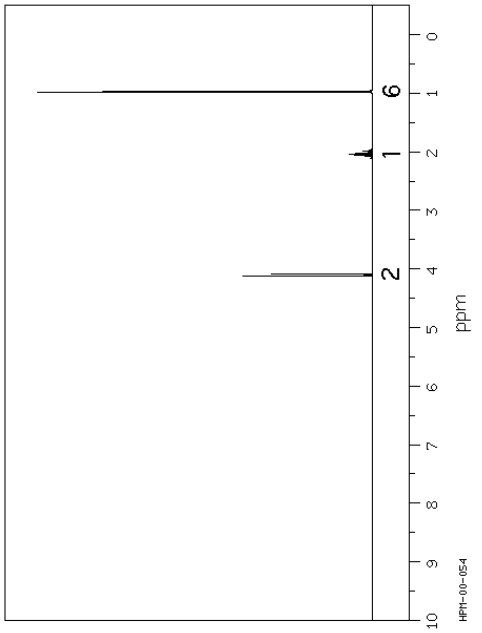
^{1}H NMR

ppm

4.118
4.096

2.113
2.091
2.069
2.046
2.024
2.002
1.98

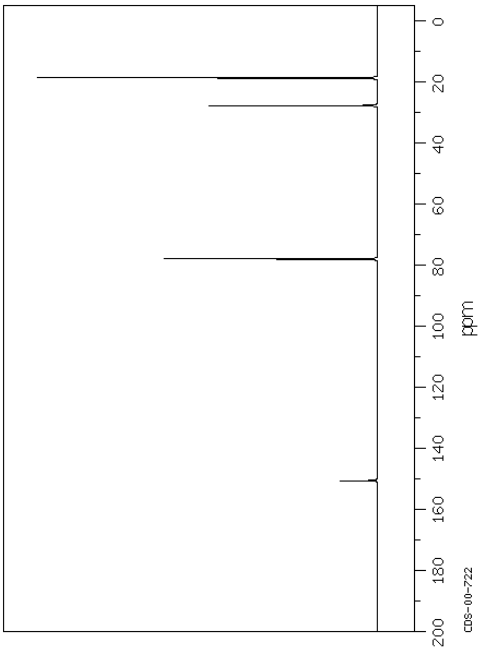
0.992
0.97



^{13}C NMR

ppm

142
78
27
19



a. (4 pts.) Assign the peaks in the ^{1}H NMR spectrum; that is, label the protons with letters and label their respective peaks in the ^{1}H NMR spectrum with the same letter.

b. (4 pts.) Assign the peaks in the ^{13}C NMR spectrum; that is, number the C atoms and label their respective peaks in the ^{13}C NMR spectrum with the same number.

c. (4 pts.) Why are there four different types of C atoms in the molecule even though the molecule actually contains five C atoms.

d. (2 pts.) Why does the ^{13}C NMR have four peaks whereas the ^{1}H NMR only has there?