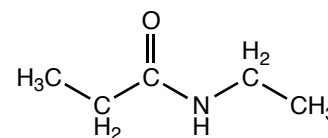
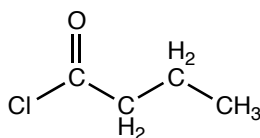
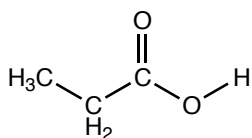
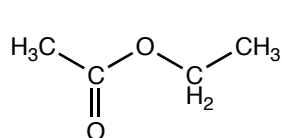
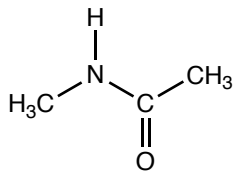


1. (12 pts) The molar mass of 2-bromopentane is 151.05 g/mol, but in the mass spectrum, there is only a tiny peak at m/z of 151.01. There are larger peaks present at m/z 150.00 and 152.00. Explain why there are larger peaks at m/z 150.00 and 152.00, a small peak at m/z 151.01, and no peak at m/z 151.05. 1. _____
2. _____
3. _____
4. _____
5. _____
2. (6 pts.) If the molecular ion $[C_6H_{12}]^+$ that creates a signal at m/z 84.09 is assigned an intensity of 100%, what would the intensity of the $m+1$ peak at m/z of 85.10 be? 6. _____
7. _____
8. _____
9. _____
3. (10 pts.) In an infrared spectrum of an alcohol, the peak associated with the stretching of the O-H bond is typically broad and the peaks associated with the C-H bonds of the alcohol are typically sharp. Explain why the OH peaks are broad and by the C-H peaks are sharp. 10. _____
11. _____

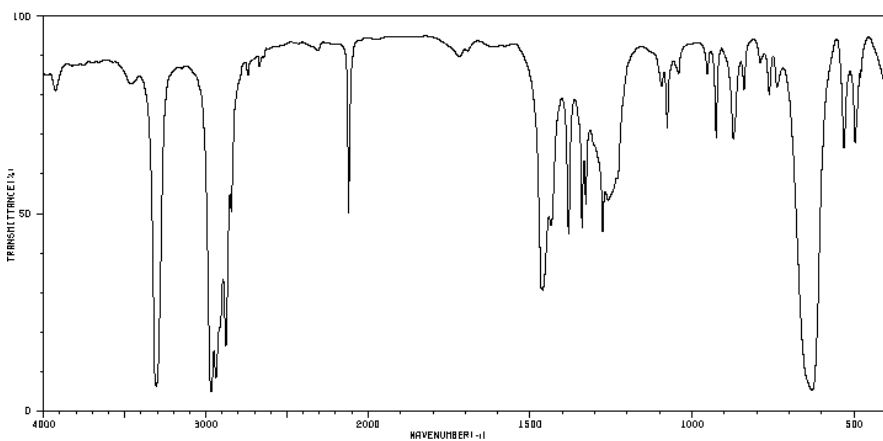
4. (12 pts.) Provide names for the functional groups in the following molecules.



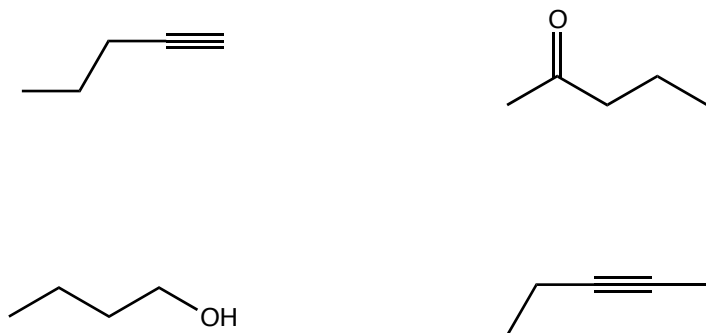
5. (8 pts.) Draw a resonance contributor for the following structure and briefly explain why the C=O stretching frequency of an amide is lower than the stretching frequency of a ketone.



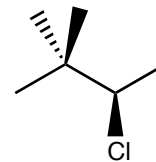
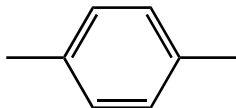
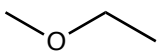
6. (a. 4 pts.) Circle the molecule that produced the following spectrum, (b. 9 pts.) briefly explain why structures were ruled out, and (c. 3 pts.) briefly explain why your choice is the correct one.



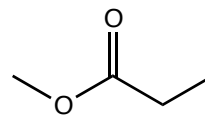
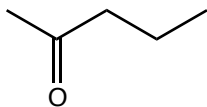
wave number (cm ⁻¹)	% transmittance	wave number (cm ⁻¹)	% transmittance
3928	79	1328	50
3457	79	1276	43
3307	6	1259	52
2968	4	1095	79
2938	7	1077	68
2876	16	1041	81
2843	49	954	81
2741	81	925	65
2670	84	872	68
2120	47	840	79
1718	86	791	84
1466	29	762	77
1450	29	730	79
1436	44	630	5
1381	43	532	54
1340	44	497	66



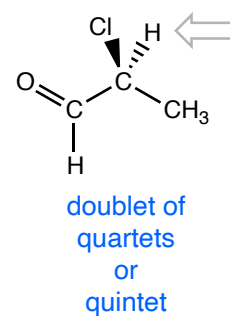
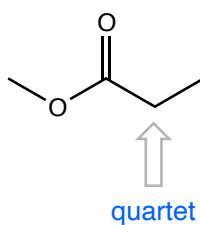
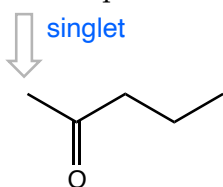
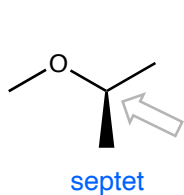
7. (9 pts.) Determine the number of peaks that would be seen in the ¹H NMR spectrum for the following molecules.



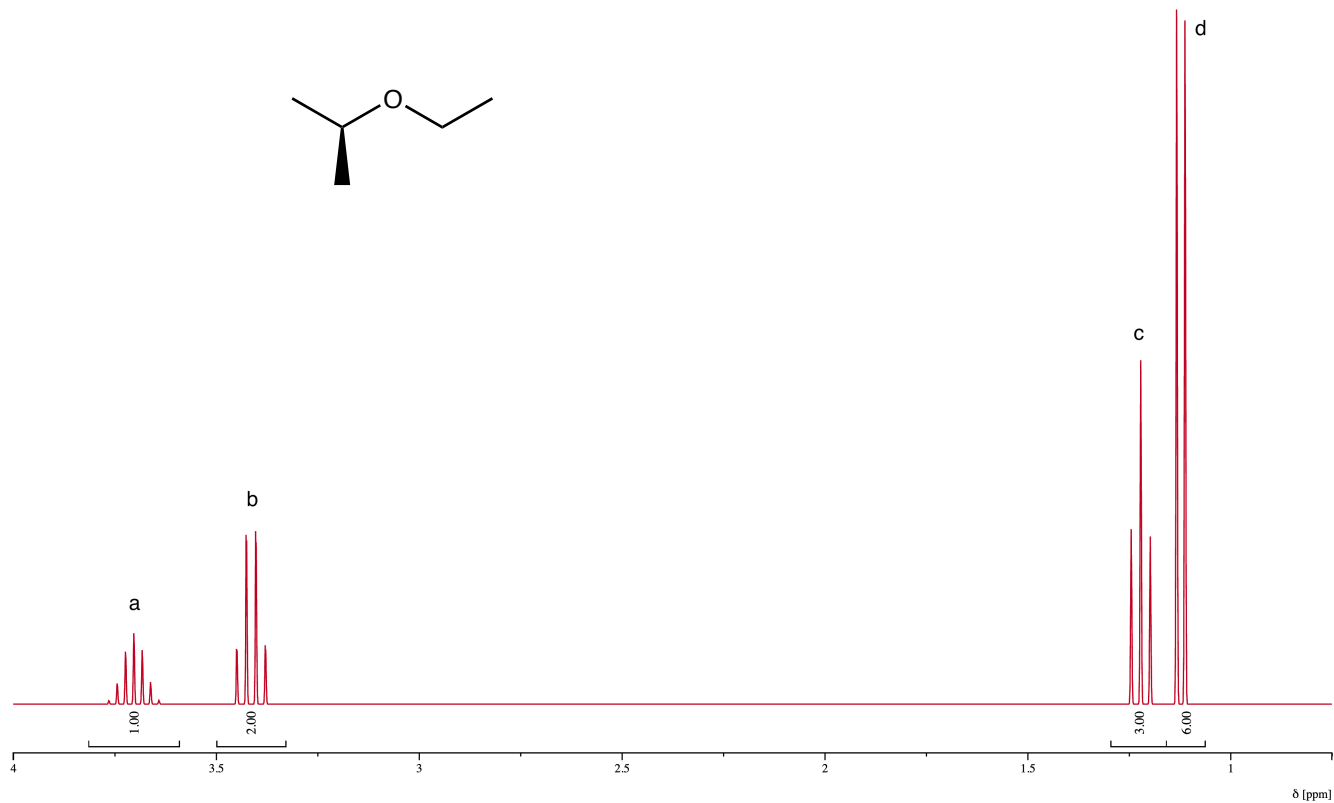
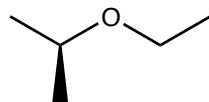
8. (9 pts.) Determine the relative positions of the peaks in the ^1H NMR spectrum; that is, label the protons alphabetically starting with the proton(s) that resonate at the highest frequency (appear farthest to the left in the NMR spectrum).



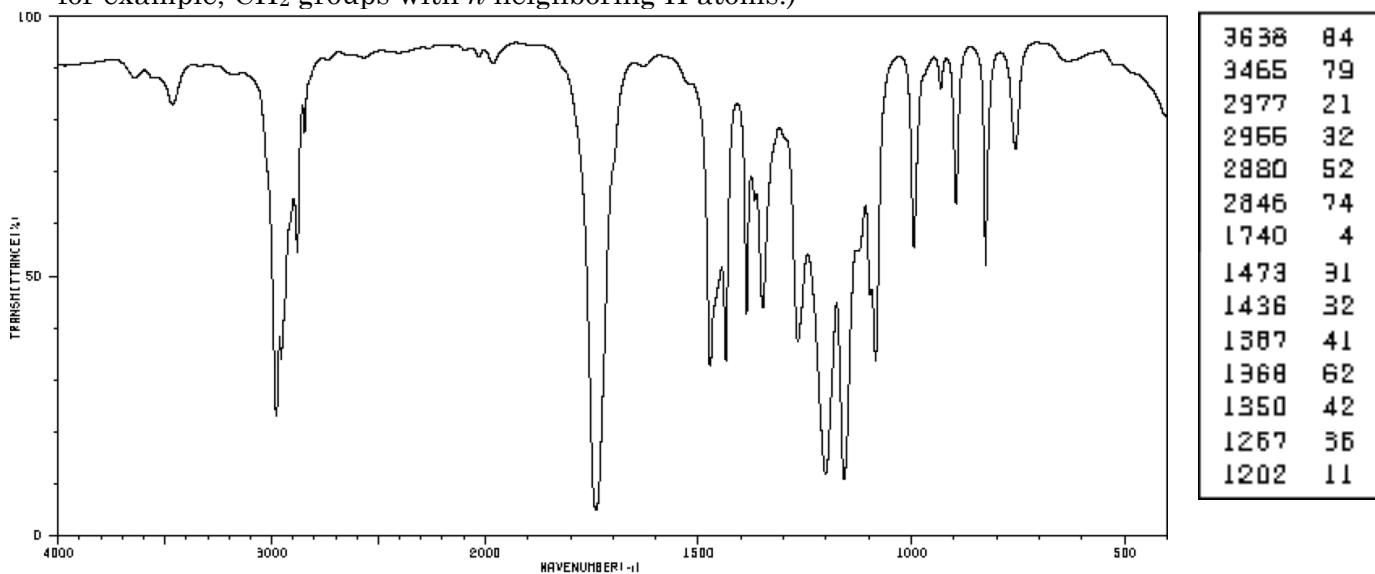
9. (8 pts.) Determine the multiplicity (the patterns: singlet, doublet, triplet, etc.) of the peaks associated with the indicated protons.



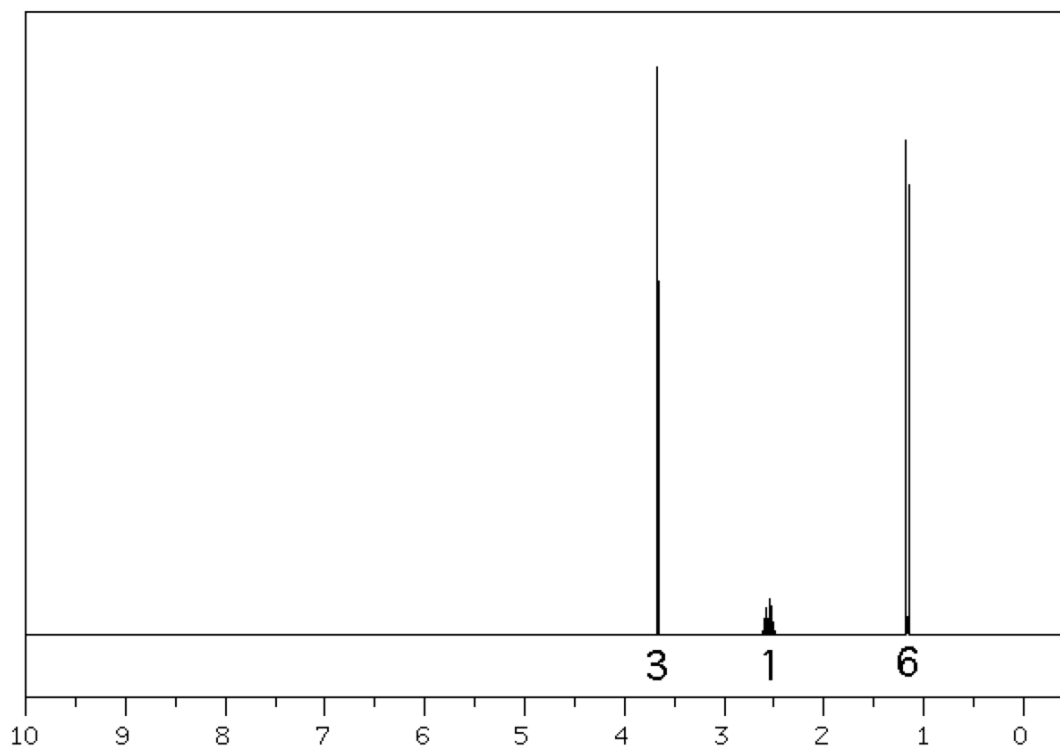
10. (12 pts.) Assign the peaks to the hydrogen atoms that are giving rise to the peaks. In other words, label the hydrogen atoms on the molecule with the labels next to the peaks in the NMR spectrum.

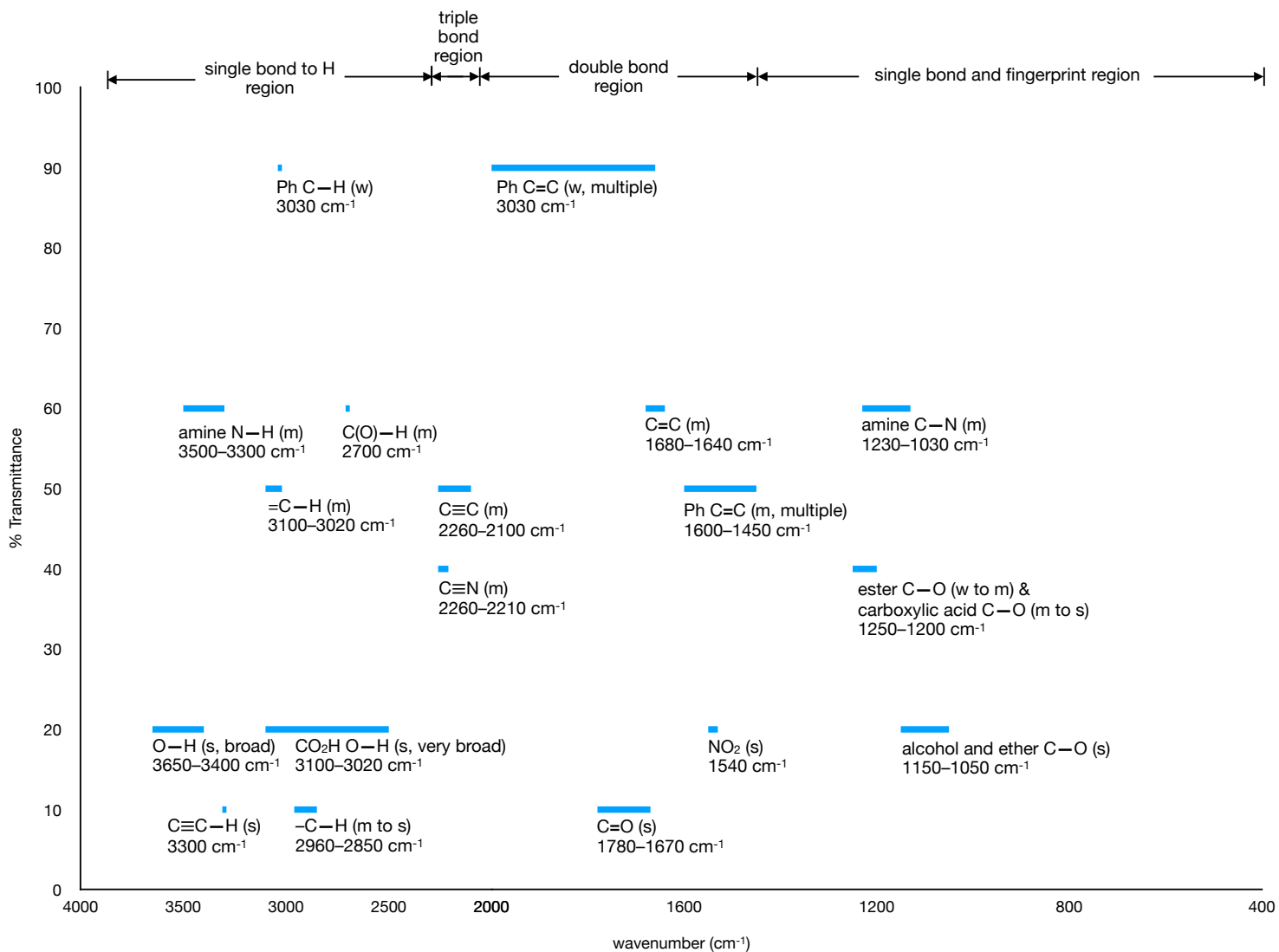


11. A molecule with the formula $C_5H_{10}O_2$ produced the following IR and 1H NMR spectra. Based on the spectral data provided below (**a. 10 pts.**) determine the structure of the unknown (**b. 4 pts.**) identify/label two peaks in the IR spectrum, and (**c. 4 pts.**) unambiguously assign the peaks in the 1H NMR spectrum. That is, label each peak in the 1H NMR spectrum alphabetically starting with an "a" at the left end of the spectrum and label the protons on your structure with the corresponding letter. (Remember, you can earn partial credit for identifying parts of the molecule; for example, CH_2 groups with n neighboring H atoms.)



ppm	height
3.669	1000
2.627	5
2.604	28
2.581	68
2.557	92
2.534	72
2.511	31
2.488	5
1.182	994
1.158	957



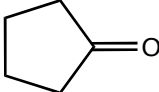


Additional information for analyzing C=O stretches:

amide: R(C=O)NH₂ < 1700

acid: RC(=O)OH 1710 usually broad for a C=O

ketone: RC(=O)R 1715, resonance stabilized ketone R=CHC(=O)R 1690

strained ketone:  1750

aldehyde: RC(=O)H 1730, resonance stabilized aldehyde R=CHC(=O)H 1705

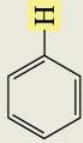
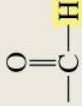

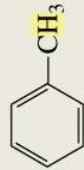

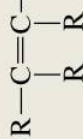
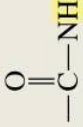
ester: RC(=O)OR 1735, resonance stabilized ester R=CHC(=O)OR 1715.

Additional information for analyzing C–H stretches:

If sp³ C–H stretch at < 3000 cm⁻¹ then look around 1400, sp³ C–H bend is at 1430 and if peak at 1380 also present then sp³ C–H is CH₃.


If sp² C–H stretch at > 3000 cm⁻¹, and not benzene gives rise to bending vibrations from 1000–600.

Table 14.1 Approximate Values of Chemical Shifts for ^1H NMR^a

Type of proton	Approximate chemical shift (ppm)	Type of proton	Approximate chemical shift (ppm)
$(\text{CH}_3)_4\text{Si}$	0		6.5–8
$-\text{CH}_3$	0.9		9.0–10
$-\text{CH}_2-$	1.3	$\text{I}-\text{C}-\text{H}$	2.5–4
$-\text{CH}-$	1.4	$\text{Br}-\text{C}-\text{H}$	2.5–4
$-\text{C}=\text{C}-\text{CH}_3$	1.7	$\text{Cl}-\text{C}-\text{H}$	3–4
	2.1	$\text{F}-\text{C}-\text{H}$	4–4.5
	2.3	RNH_2	Variable, 1.5–4
$-\text{C}\equiv\text{C}-\text{H}$	2.4	ROH	Variable, 2–5
$\text{R}-\text{O}-\text{CH}_3$	3.3	ArOH	Variable, 4–7
$\text{R}-\text{C}=\text{CH}_2$	4.7		Variable, 10–12
	5.3		Variable, 5–8

^aThe values are approximate because they are affected by neighboring substituents.

Table 14.4 Approximate Values of Chemical Shifts for ^{13}C NMR

Type of carbon	Approximate chemical shift (ppm)	Type of carbon	Approximate chemical shift (ppm)
$(\text{CH}_3)_4\text{Si}$	0	$\text{C}-\text{I}$	0–40
$\text{R}-\text{CH}_3$	8–35	$\text{C}-\text{Br}$	25–65
$\text{R}-\text{CH}_2-\text{R}$	15–50	$\text{C}-\text{Cl}$	35–80
$\text{R}-\text{CH}-\text{R}$	20–60	$\text{C}-\text{N}$	40–60
$\text{R}-\text{C}-\text{R}$	30–40	$\text{C}-\text{O}$	50–80
$\equiv\text{C}$	65–85	$\text{R}-\text{C}=\text{O}$	165–175
$=\text{C}$	100–150	$\text{R}-\text{C}=\text{O}$	165–175
	110–170	$\text{R}-\text{C}=\text{O}$	175–185
		$\text{R}-\text{C}=\text{O}$	190–200
		$\text{R}-\text{C}=\text{O}$	205–220