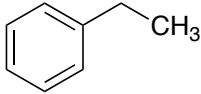
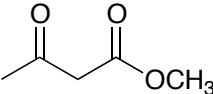
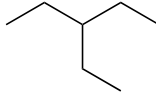
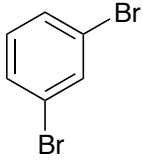
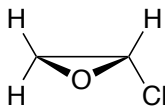
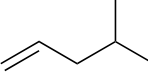
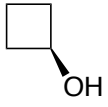
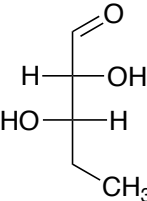
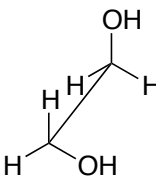
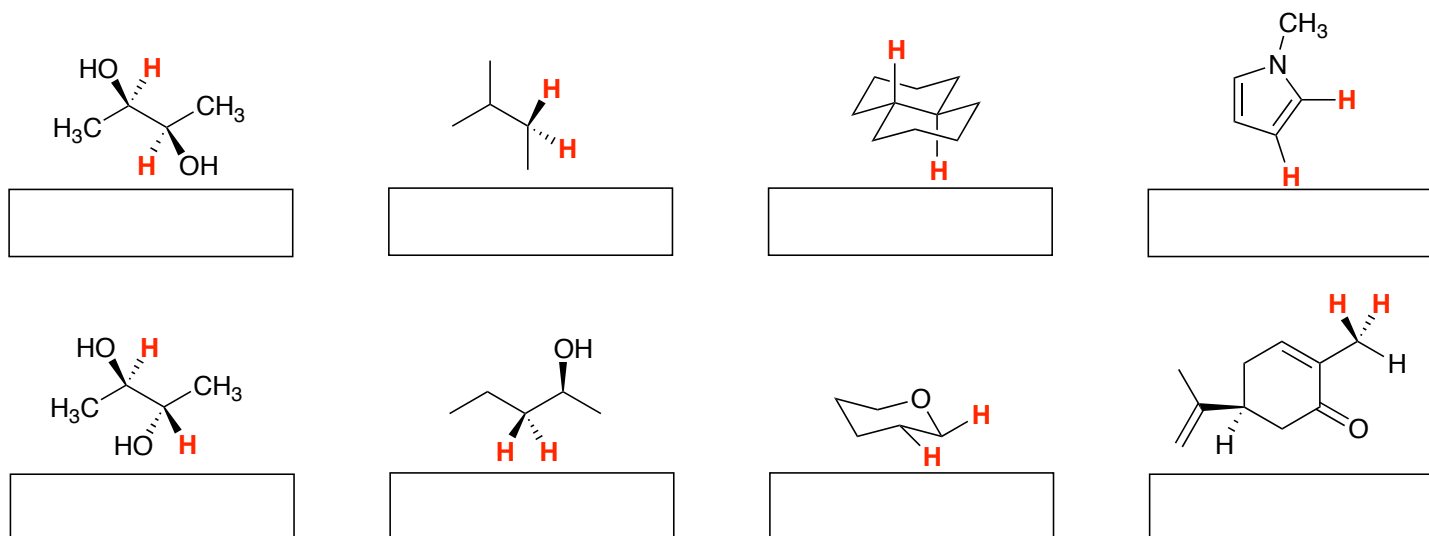


Completion (6 pts)		Name	
Random Sample(s) (4 pts)		BID	
Total (10 pts)		Section-CRN	
Additional Recommended Problems from McMurray (8 th Ed.)			

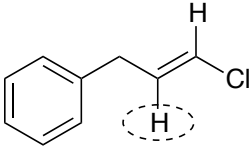
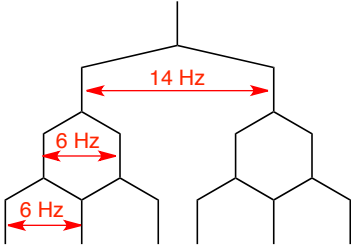
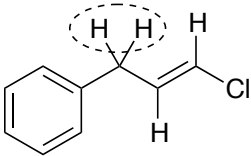
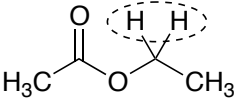
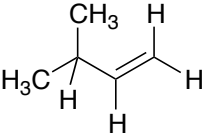
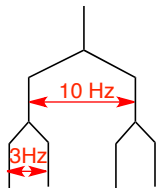
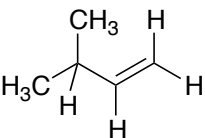
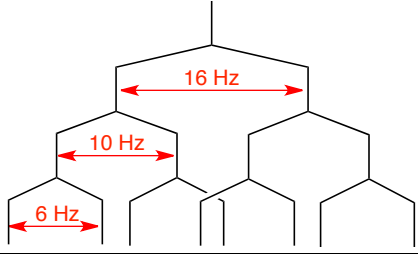
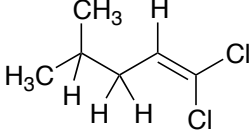
1. For each molecule, list the number of signals you'd expect to see in the ¹H-NMR and ¹³C-NMR spectra. Assume no signals overlap.

	¹ H	¹³ C		¹ H	¹³ C		¹ H	¹³ C
								
								
								

2. Label the bold H atoms in each molecule as homotopic, enantiotopic, diastereotopic or heterotopic. *Careful! Do the equivalency tests to be sure.*



3. Fill in the missing fields in the table below to complete each row. You may need to circle the appropriate set of H-atoms in the molecule for some entries. The first row is completed as an example.

Signal (Circled)	Multiplicity Name	Multiplicity Abbreviation	Coupling Constant(s)	Splitting Tree
	douplet of triplets	dt	$J = 14, 6 \text{ Hz}$	
			$J = 8 \text{ Hz}$	
			$J = 5 \text{ Hz}$	
 <p><i>Circle appropriate Hs.</i></p>			$J = 10, 8 \text{ Hz}$	
 <p><i>Circle appropriate Hs.</i></p>			$J = 16, 10, 6 \text{ Hz}$	
 <p><i>Circle appropriate Hs.</i></p>		dd	$J = 8, 8 \text{ Hz}$	

Homework Five & Six Organic Chemistry I (223) Prof. Landrie • Spring 2013	Name	
	BID	
	Section-CRN	

4. Propose structures for compounds that fit the following ^1H NMR data.

a. $\text{C}_4\text{H}_6\text{Cl}_2$ 2.18 δ (3 H, singlet) 4.16 δ (2 H, doublet, $J = 7$ Hz) 5.71 δ (1 H, triplet, $J = 7$ Hz)	b. $\text{C}_{10}\text{H}_{14}$ 1.30 δ (9 H, singlet) 7.30 δ (5 H, singlet)
c. $\text{C}_4\text{H}_7\text{BrO}$ 2.11 δ (3 H, singlet) 3.52 δ (2 H, triplet, $J = 6$ Hz) 4.40 δ (2 H, triplet, $J = 6$ Hz)	d. $\text{C}_9\text{H}_{11}\text{Br}$ 2.15 δ (2 H, quintet, $J = 7$ Hz) 2.75 δ (2 H, triplet, $J = 7$ Hz) 3.38 δ (2 H, triplet, $J = 7$ Hz) 7.22 δ (5 H, singlet)

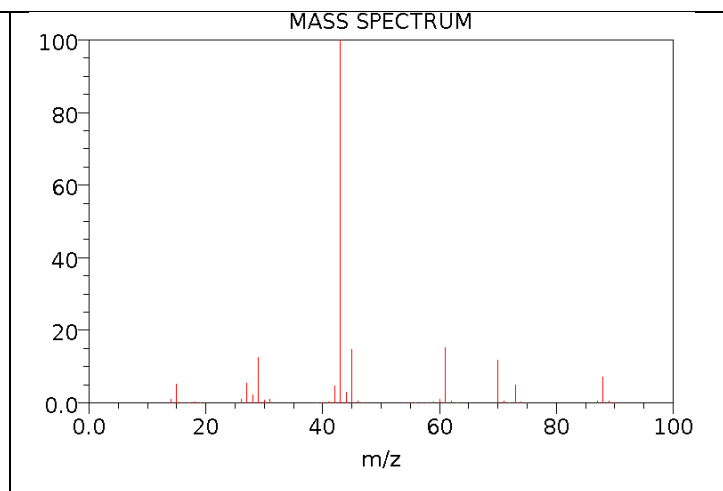
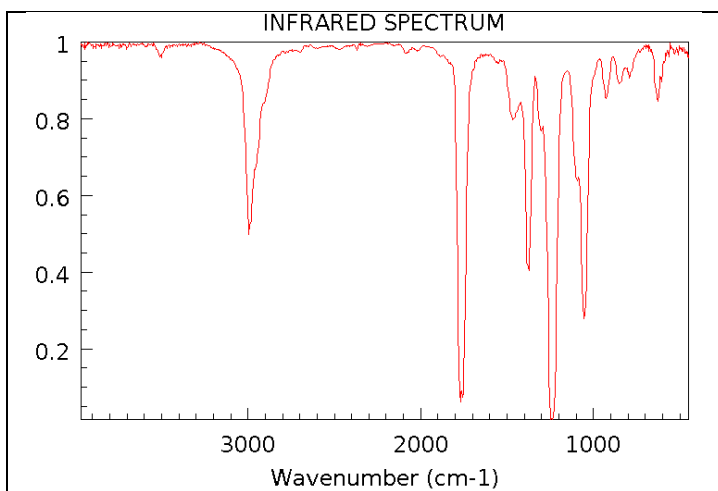
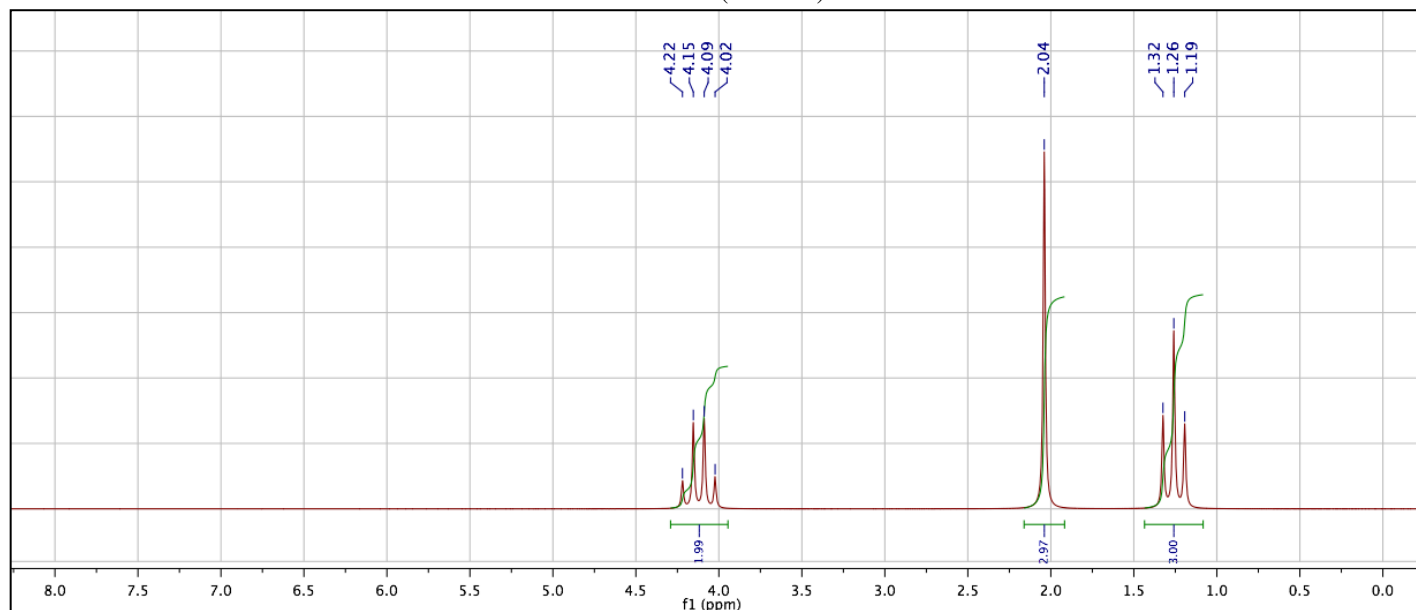
5. When measured on a spectrometer operating at 200 MHz, chloroform (CHCl_3) shows a single sharp absorption at 7.28 δ (ppm).

- How many Hertz downfield from TMS does chloroform absorb?
- How many Hertz downfield from TMS would chloroform absorb if the measurement were carried out on a spectrometer operating at 500 MHz?
- What would be the position of the chloroform absorption in δ units when measured on a 500 MHz spectrometer.

Homework Five & Six Organic Chemistry I (223) Prof. Landrie • Spring 2013	Name	
	OCC ID	
	Section CRN	

Molecular Formula:	?	Elemental Analysis:	C, 54.53%; H, 9.15%; O, 36.32%
---------------------------	---	----------------------------	--------------------------------

¹H-NMR (90 MHz)



6. Determine the structure from the data above. Show all work and analysis where possible.

7. Calculate the J-values for the quartet and triplet. Show all work.

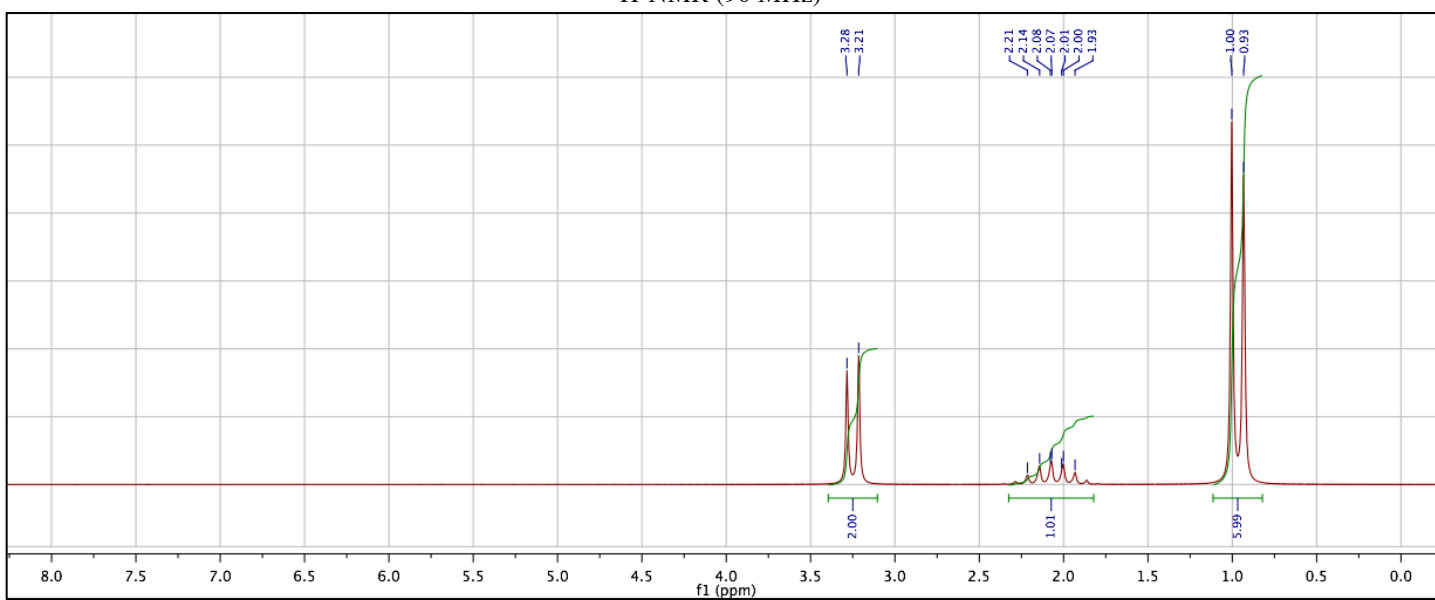
Molecular Formula:

C₄H₉Br

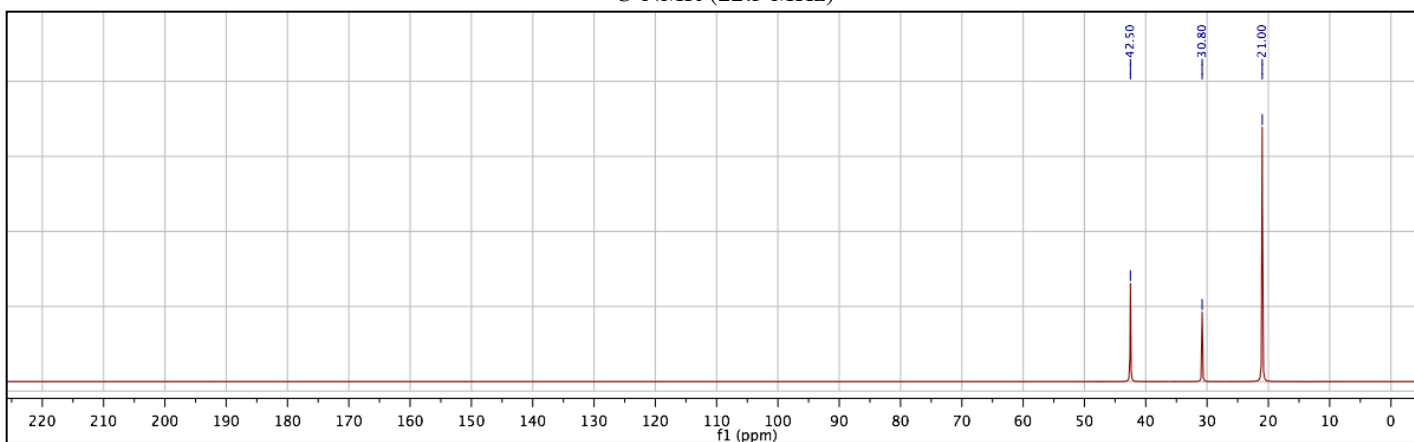
Elemental Analysis:

?

¹H-NMR (90 MHz)



¹³C-NMR (22.3 MHz)



8. Determine the structure from the data above. Show all work and analysis where possible.

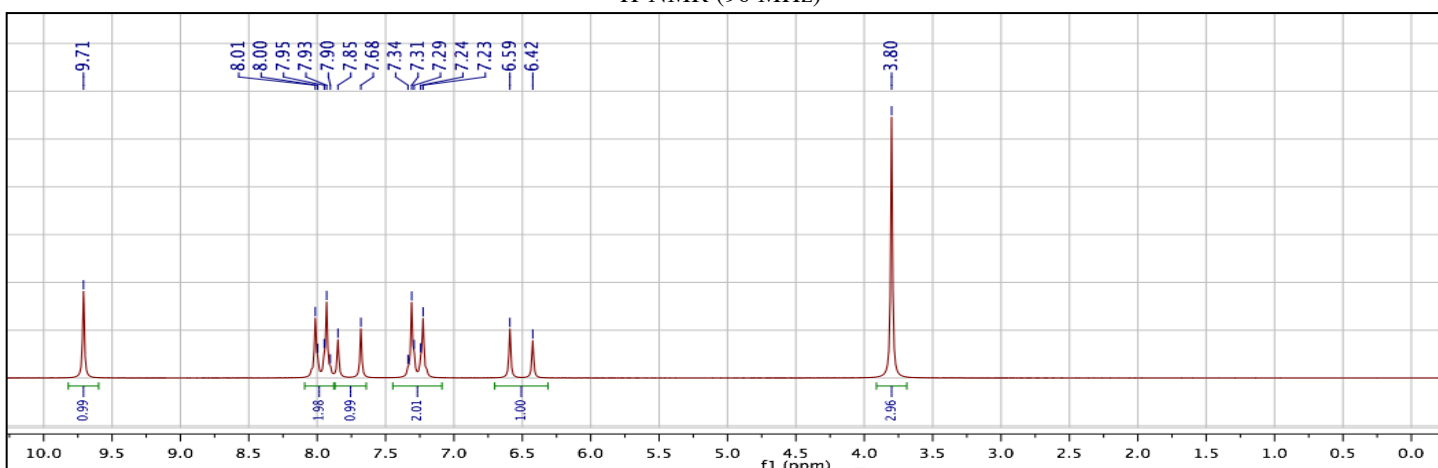
Molecular Formula:

$C_{10}H_{10}O_2$

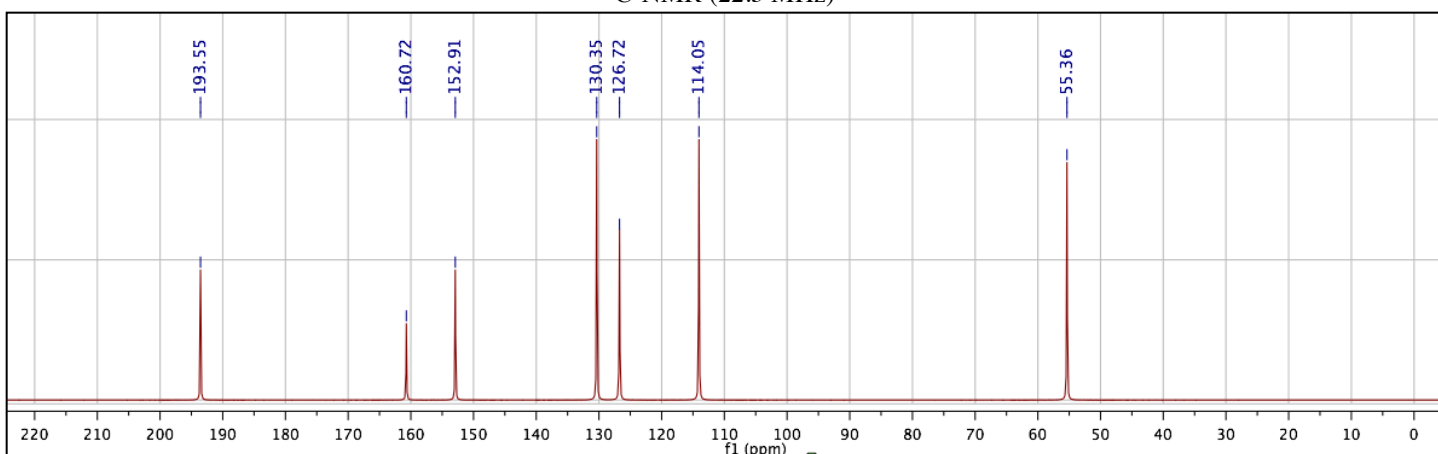
Elemental Analysis:

?

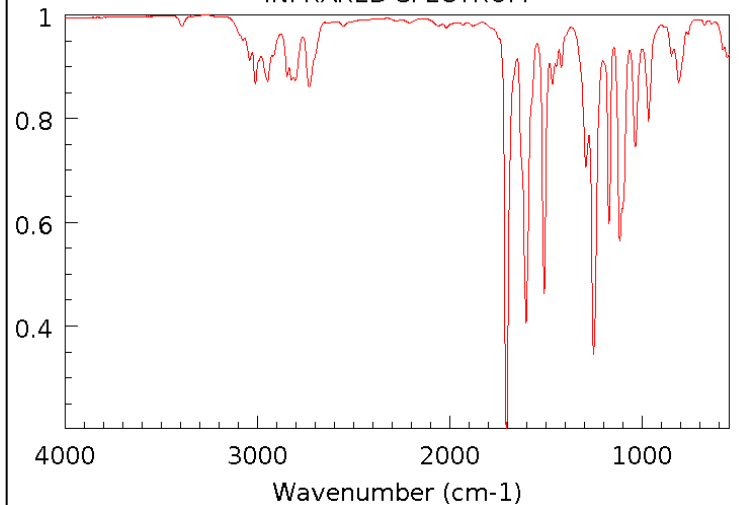
1H -NMR (90 MHz)



^{13}C -NMR (22.3 MHz)



INFRARED SPECTRUM



9. Determine the structure from the data above. Show all work and analysis where possible.

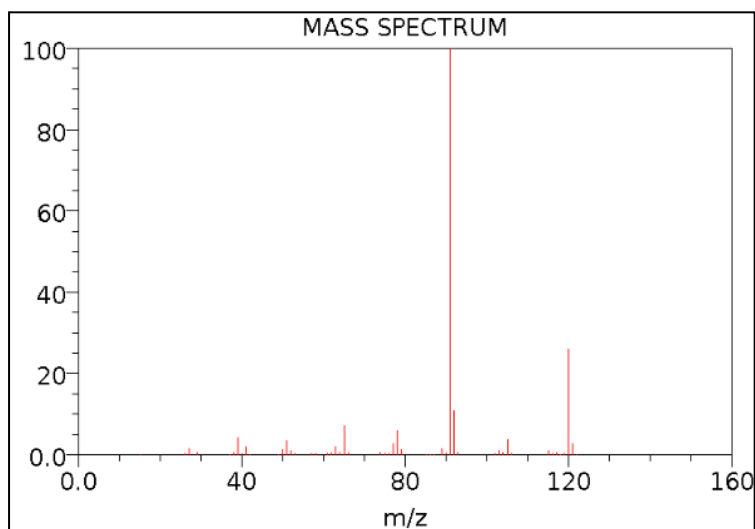
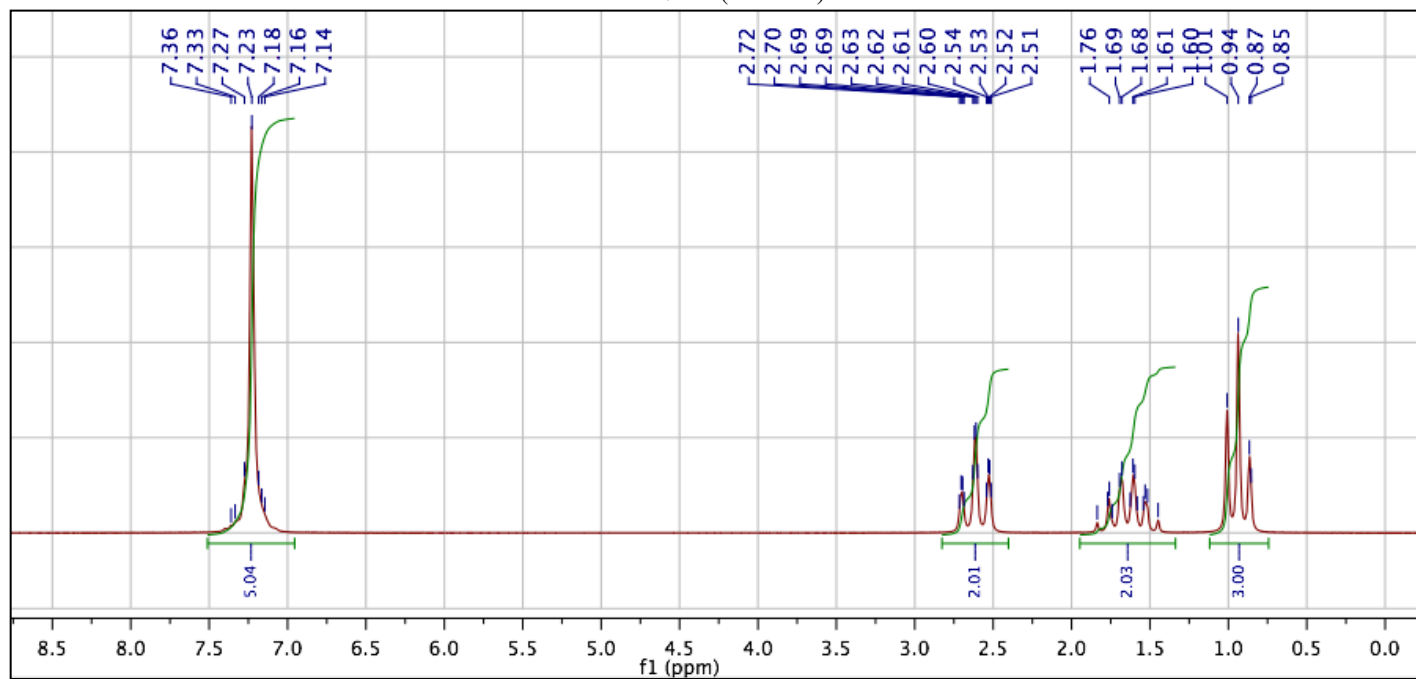
Molecular Formula:

?

Elemental Analysis:

?

$^1\text{H-NMR}$ (90 MHz)



10. Determine the structure from the data above. Show all work and analysis where possible.

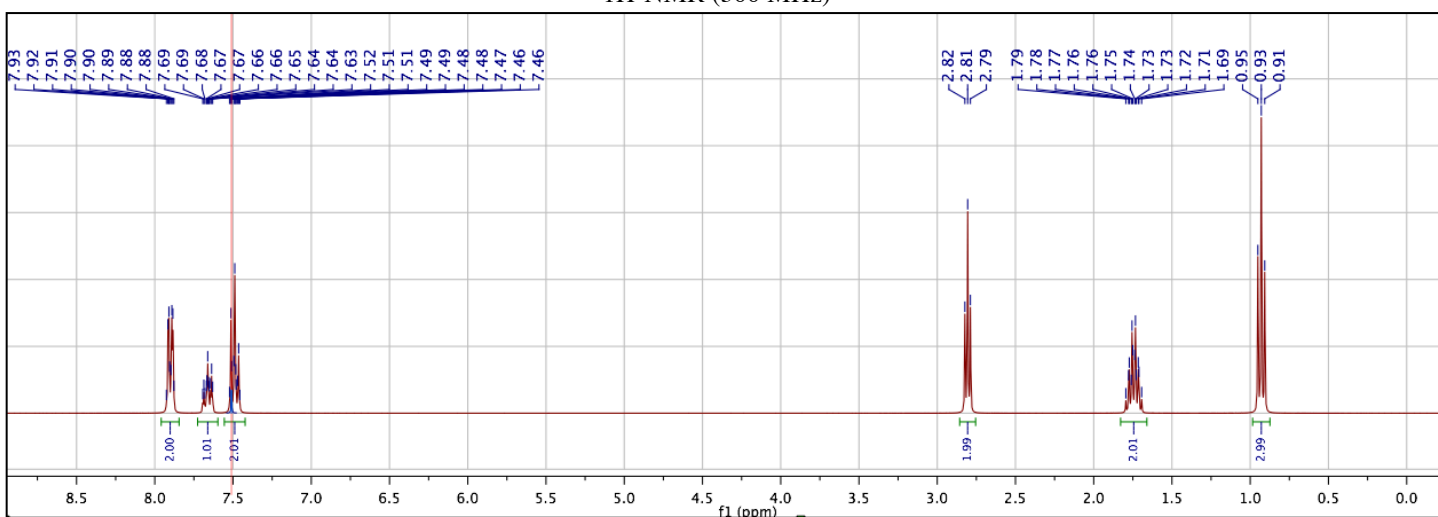
11. Draw the cation fragment that gives rise to the peak at 91 in the mass spectrum.

Molecular Formula: ?

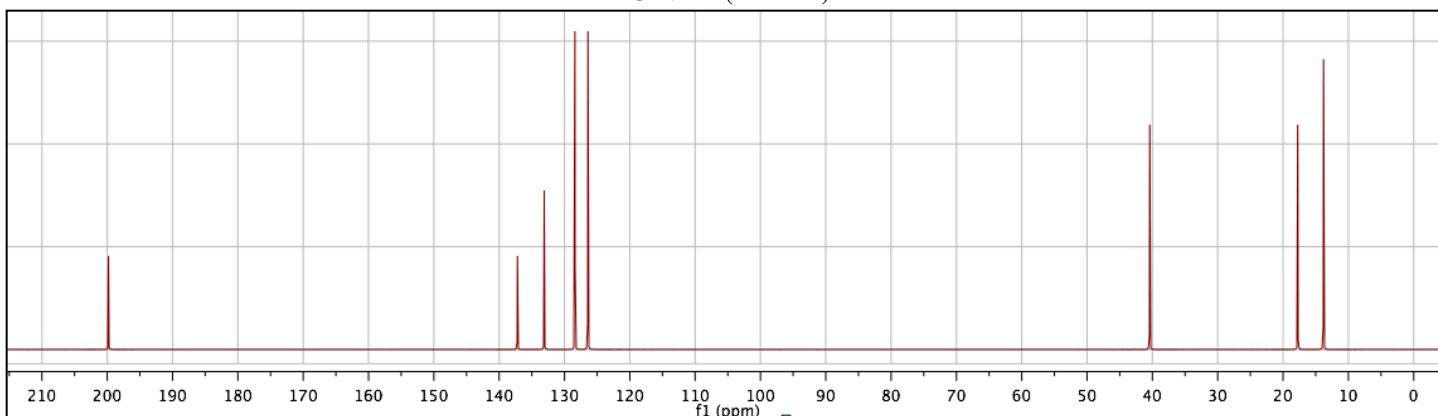
Elemental Analysis:

C (81.04%); H (8.16%); O (10.80%)

¹H-NMR (300 MHz)



¹³C-NMR (75 MHz)

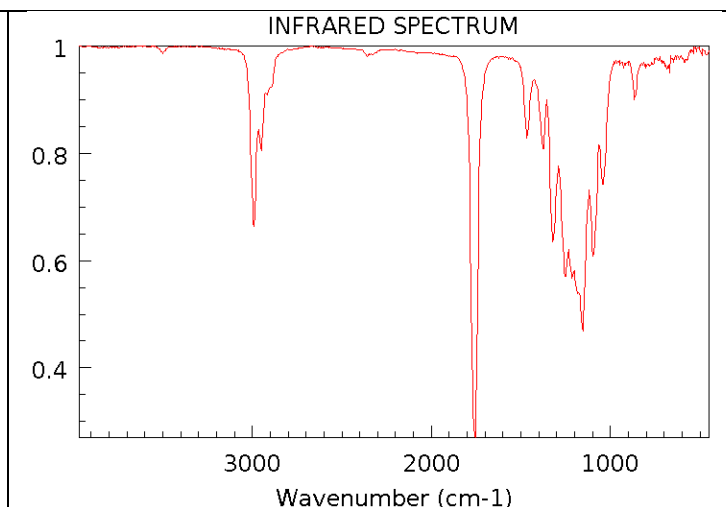
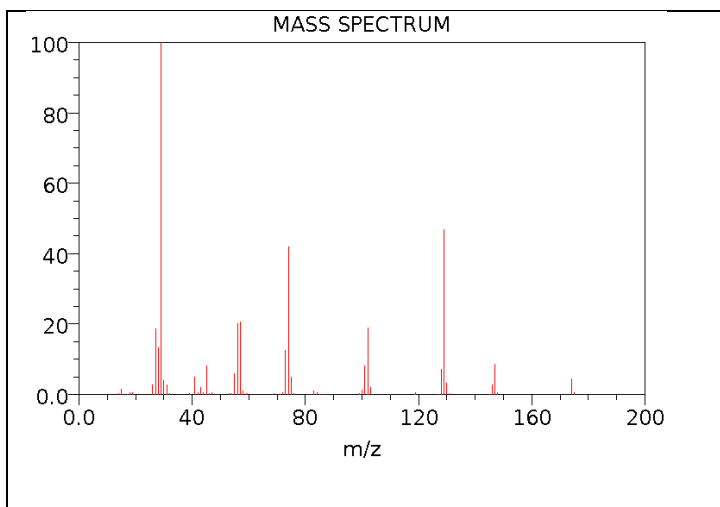
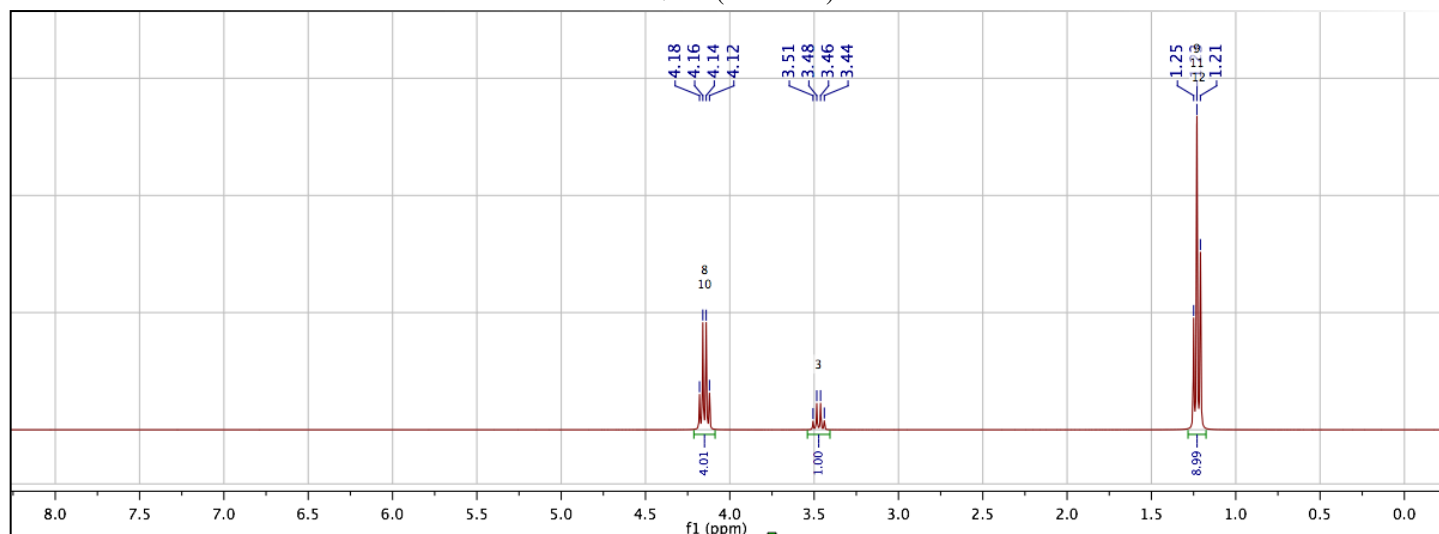


12. Determine the structure from the data above. Show all work and analysis where possible.

Homework Five & Six Organic Chemistry I (223) Prof. Landrie • Spring 2013	Name	
	OCC ID	
	Section CRN	

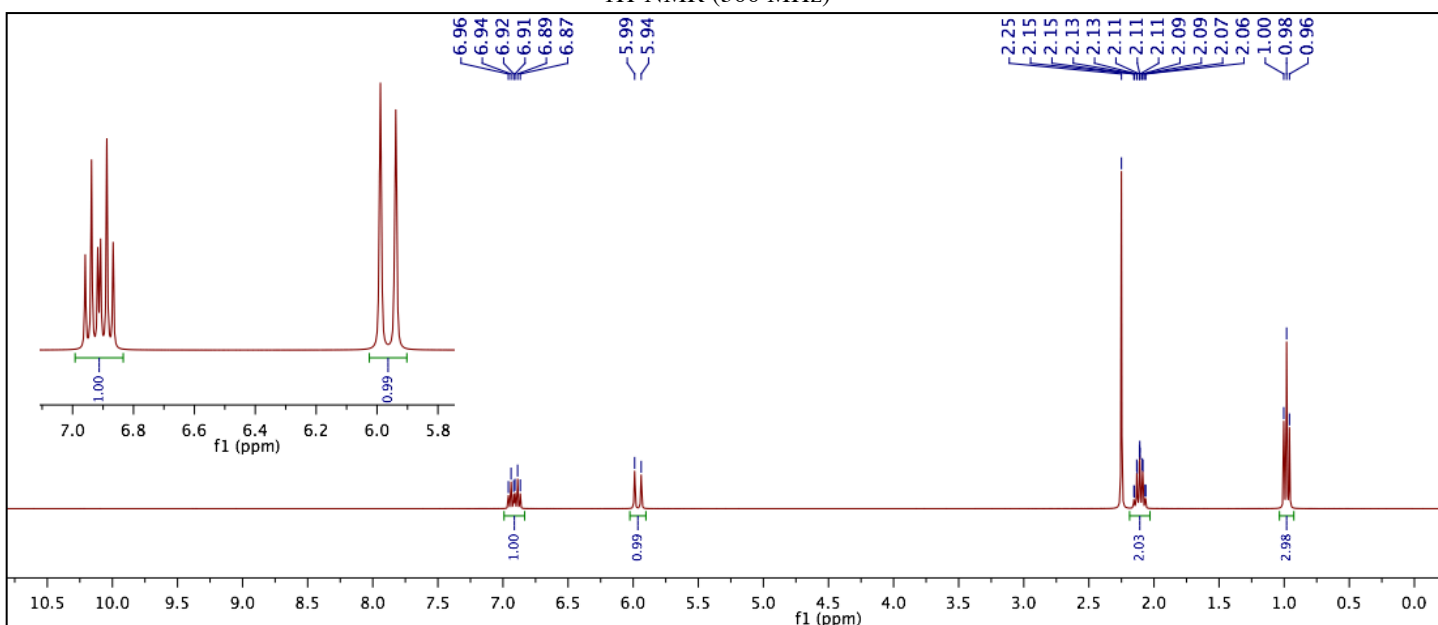
Molecular Formula:	?	Elemental Analysis:	C, 55.16%; H, 8.10%; O, 36.74%
---------------------------	---	----------------------------	--------------------------------

1H-NMR (300 MHz)

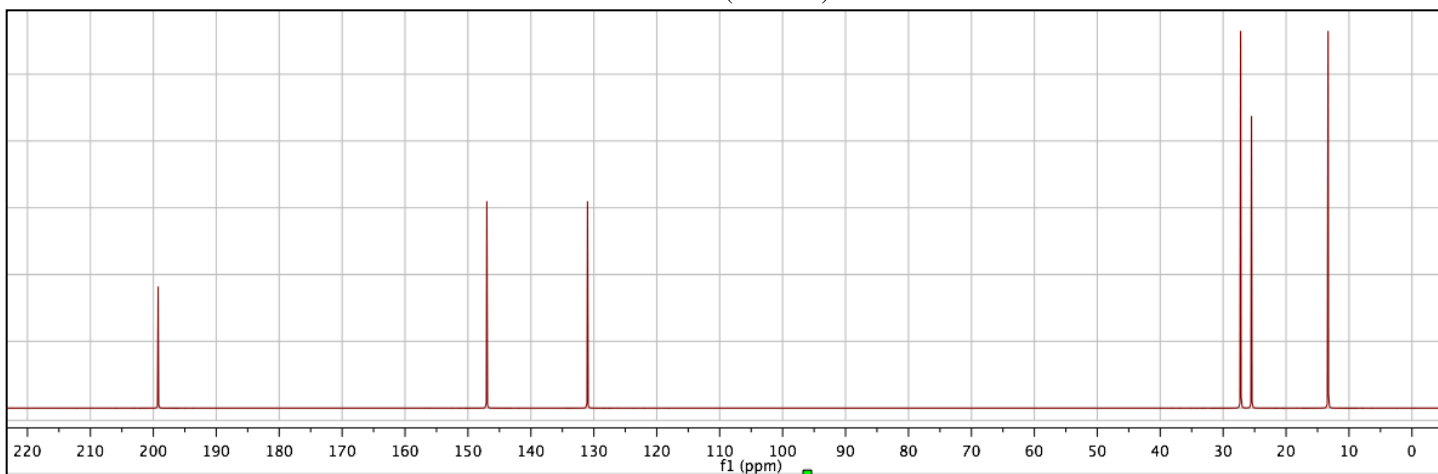


13. The molecule also shows ¹³C-NMR signals at 13.5, 13.9, 46.1, 61.2 and 170.1 ppm. Determine the structure from the data above. Show all work and analysis where possible.

1H -NMR (300 MHz)



^{13}C -NMR (75 MHz)



14. Calculate the coupling constants (there are two!) for the doublet of triplets at 6.9 ppm in the 1H -NMR. Show your work.

15. Determine the structure from the data above. Show all work and analysis where possible.