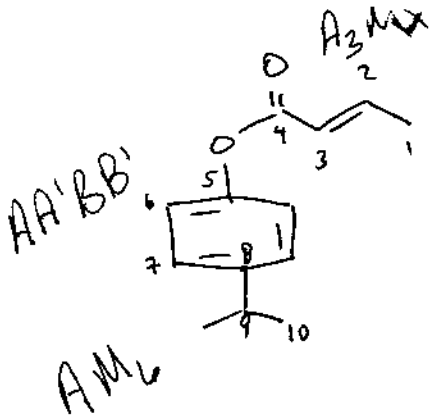
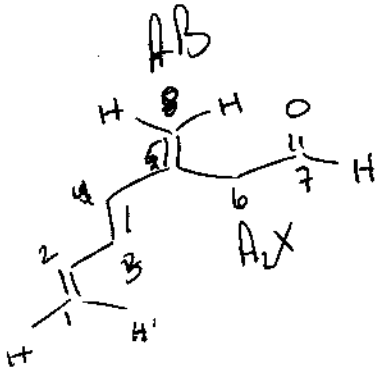
Paul's Somewhat Crude 333 Practice Final

(1) For the following Two molecules, describe using Pople notation each spin system, + roughly predict the proton + ^{13}C NMR spectra



	^{13}C	^{1}H	mult, J (Hz)
1	18	1.93	dd 8, 2
2	145	6.85	dq 14, 8
3	129	5.83	dq 14, 2
4	167	na	
5	148	na	
6	120	7.60	d, 6
7	118	7.05	d, 6
8	145	na	
9	34	2.9	sept, 8
10	24	1.3	d, 8

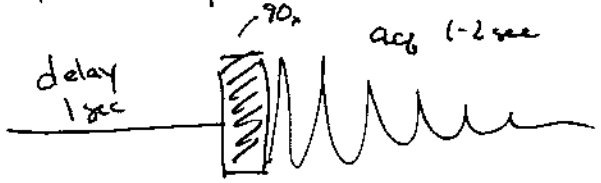


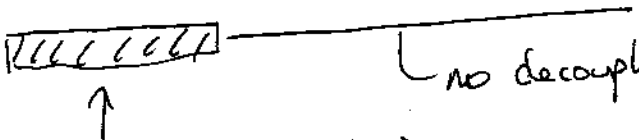
ABMXYZ

1	114	5.21 / 5.04	dd 2, 14 / dd 2, 8
2	138	6.23	ddd 8, 14, 12
3	130	6.19	dd 8, 14
4	133	6.19	d 14
5	145	na	na
6	41	3, 4	d 2
7	210	5.04	9.4 t 2
8	118	4.92 / 4.78	d 2 / d 2

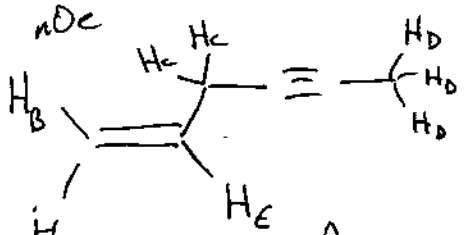
There is no #2!

(3) I have a limited quantity of a sample and need to measure $^1J + {}^2J$ C-H coupling constants. Design me a pulse sequence that will yield this data, + explain why.

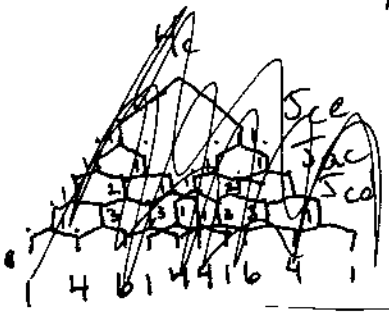


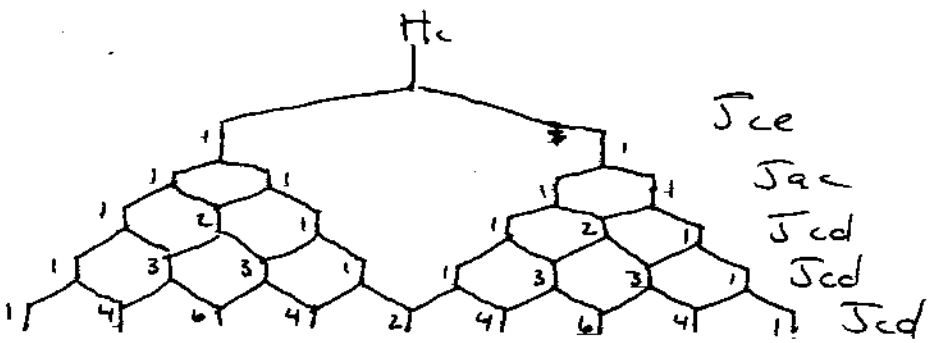


(4)

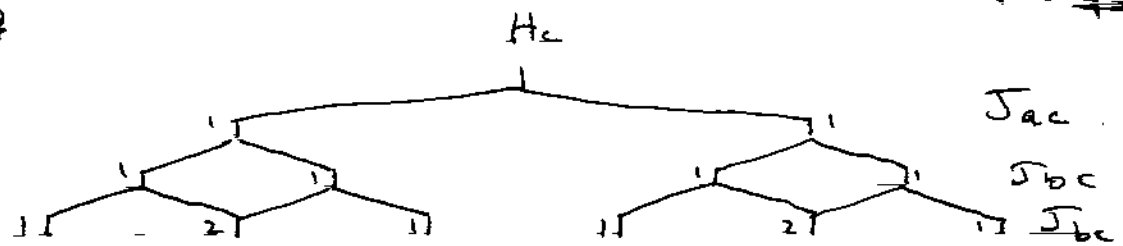


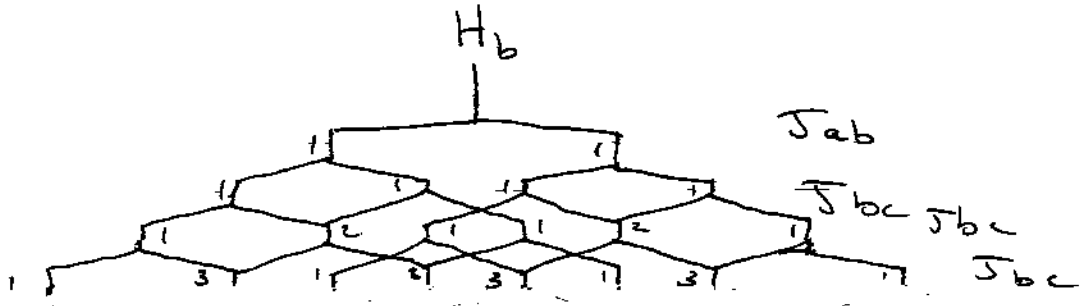
Assuming that $J_{Bc} = 0$, $J_{Ac} = 2$ Hz, $J_{Ec} = 8$ Hz, ods... + $J_{Dc} = 2$ Hz, draw a splitting diagram for H_c ONLY. Don't forget the relative intensities!

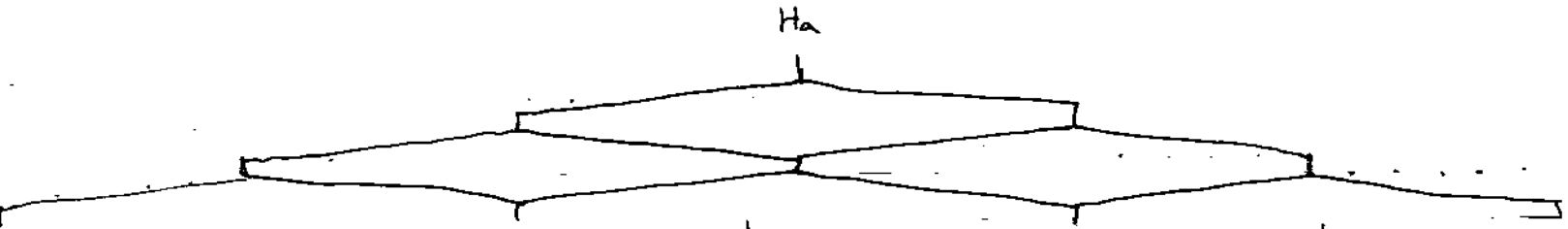




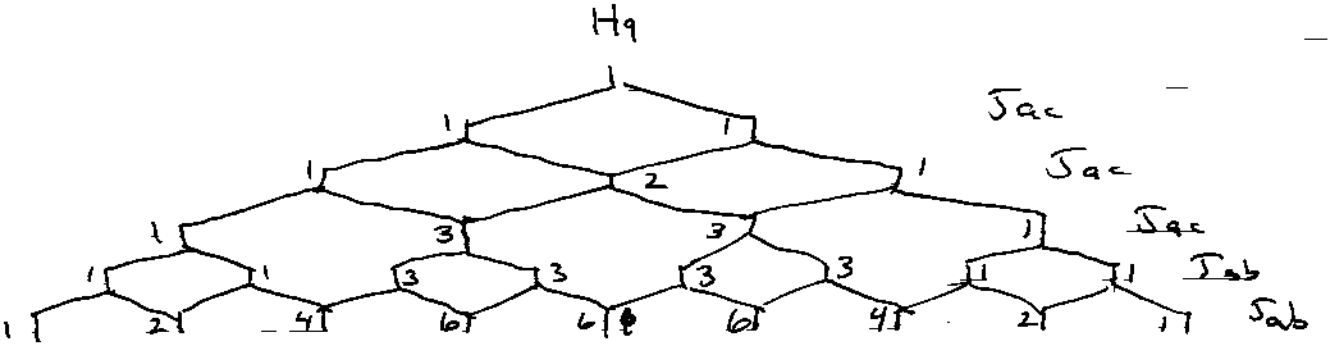
(5) For the simulated spin system on the next page, draw a stick diagram for each 1st order multiplet in the spin system. Report all J values, and fully label your stick diagrams w/ J values + relative intensities.



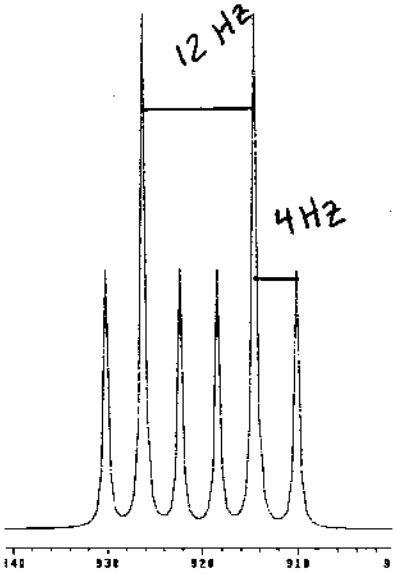




ok, I have to cut down by $\frac{1}{2}$

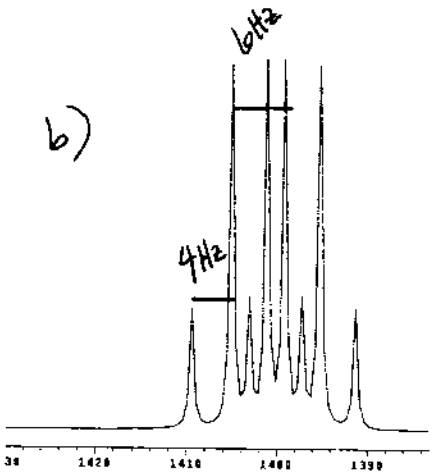


c)



dt

b)



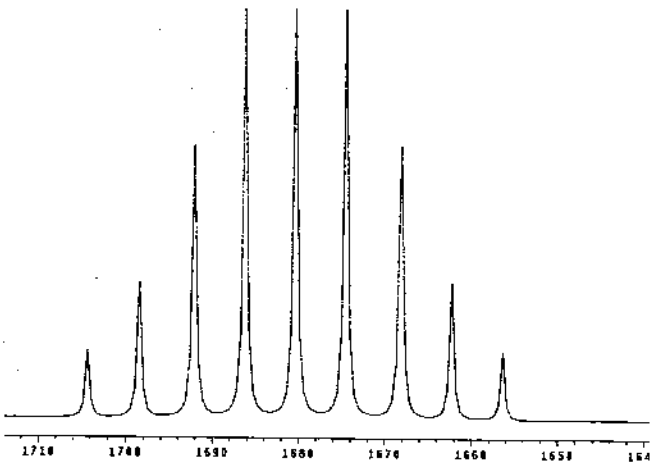
d_J

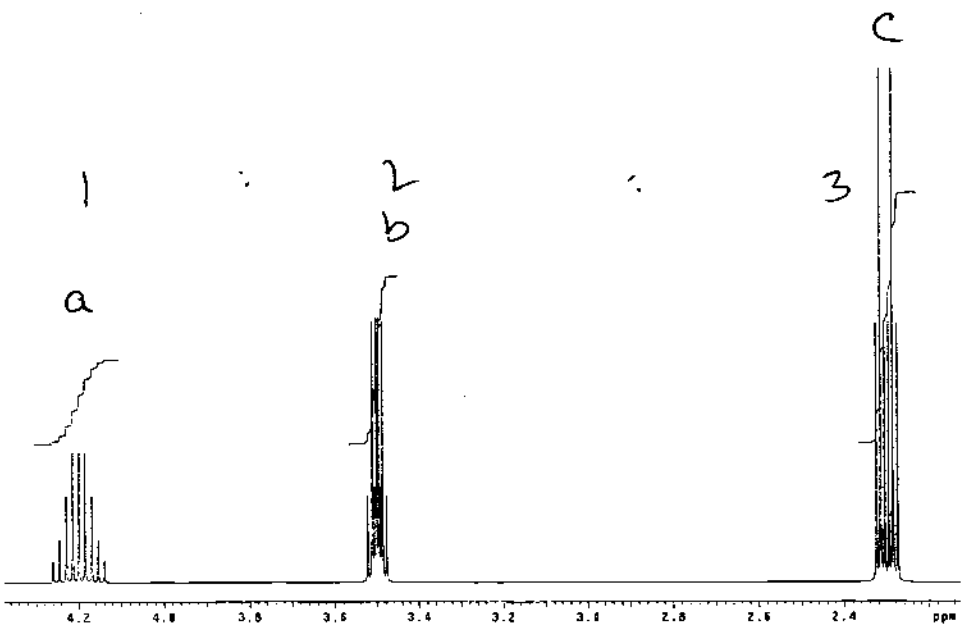
$J_{cb} = 4Hz$

$J_{ac} = 12Hz$

$J_{ab} = 6Hz$

a)





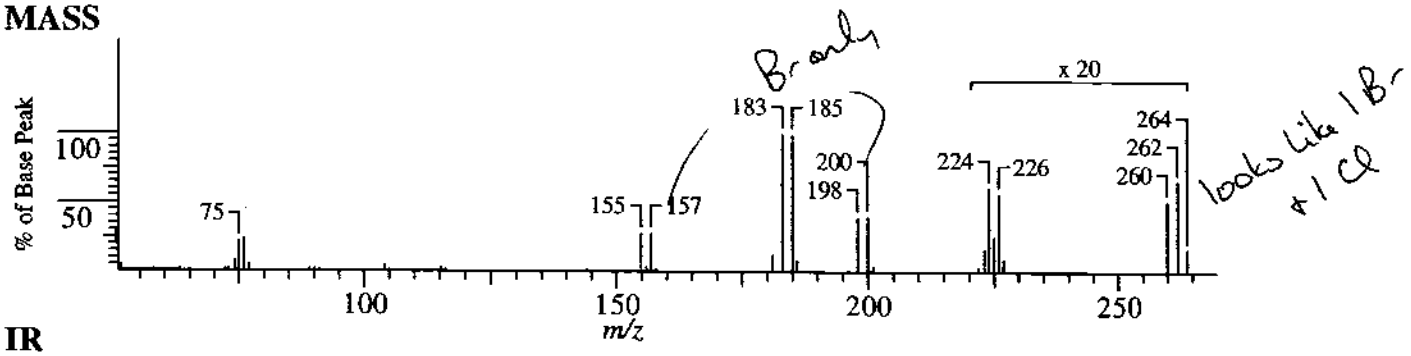
(6) The next page is a Field-type problem (well, actually it is a Field problem...). Do the usual, + show lots of work + analysis.

see page

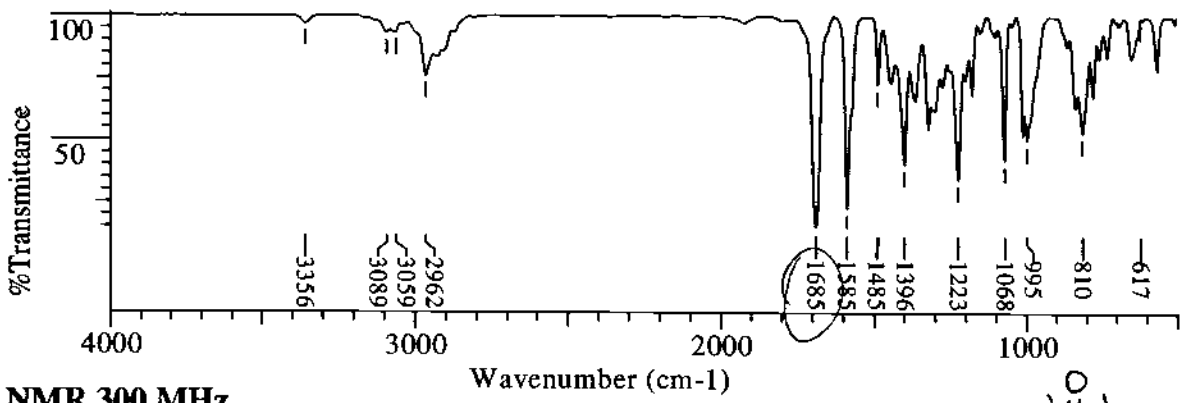
(7) The ~~page~~ page after that is a Silverstein problem with no molecular formula. Do the same as the above

see page

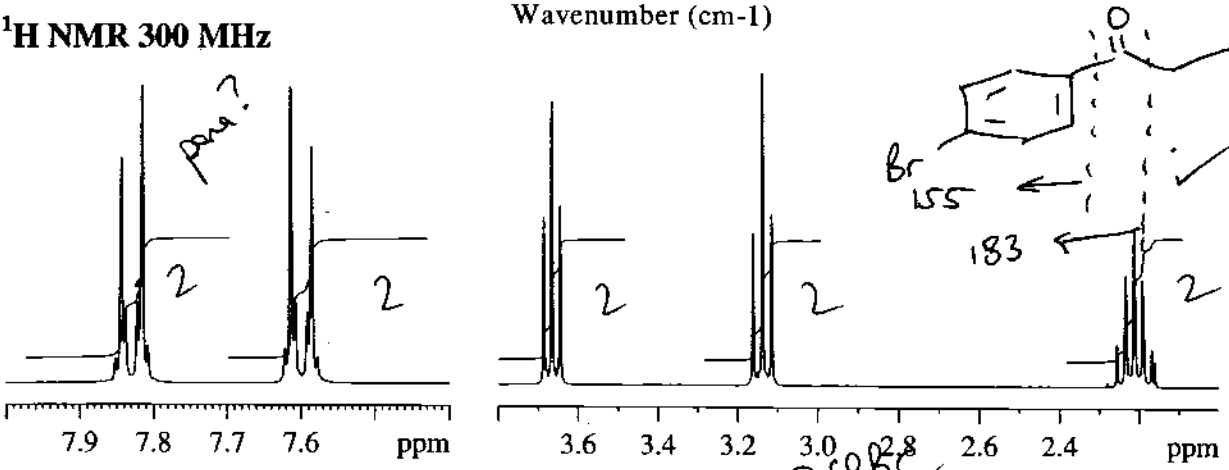
MASS



IR



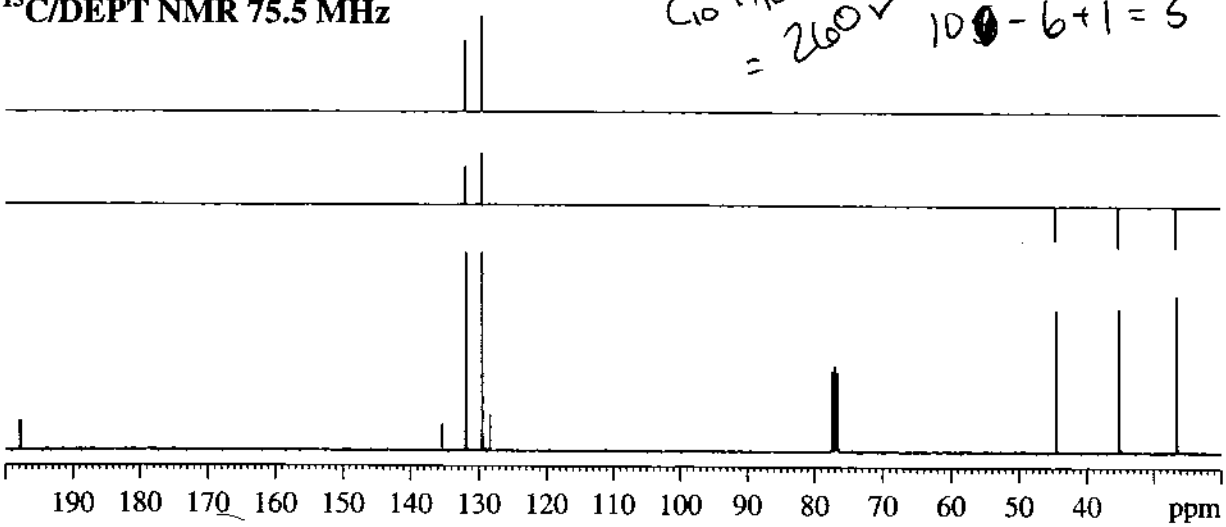
^{1}H NMR 300 MHz

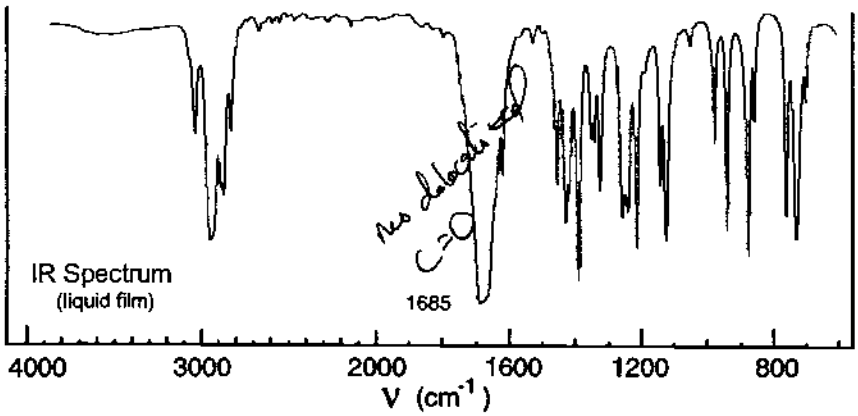


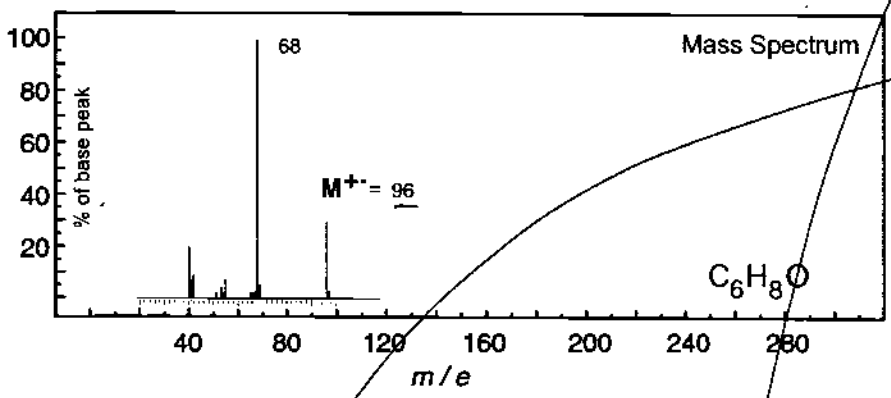
^{13}C/DEPT NMR 75.5 MHz

$C_{10}H_{10}OClBr$
$= 260$ ✓

$10 - 6 + 1 = 5$





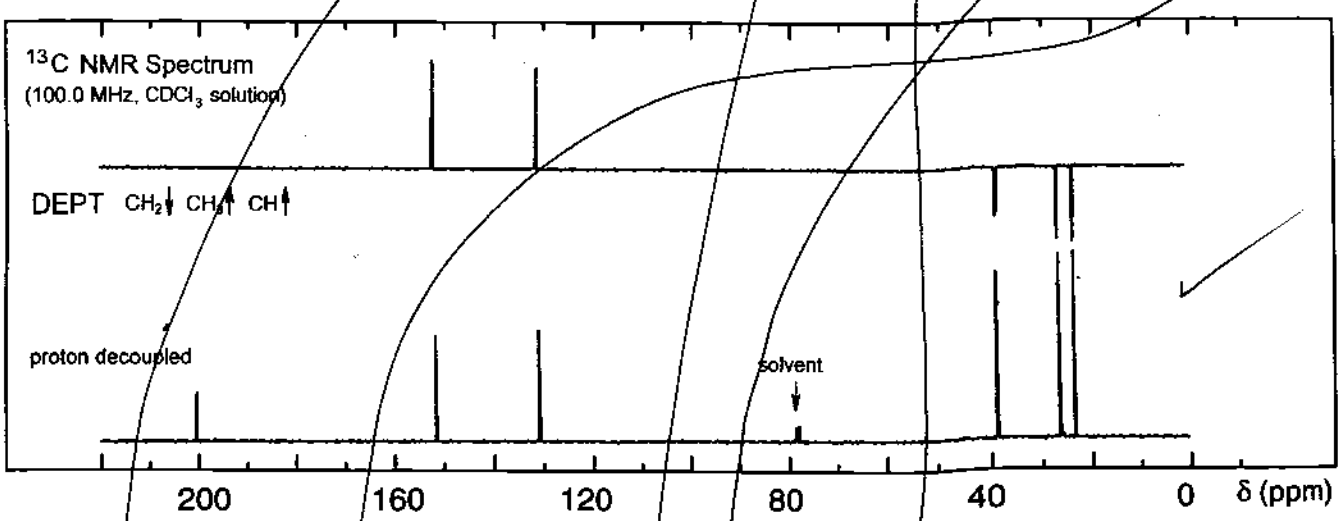


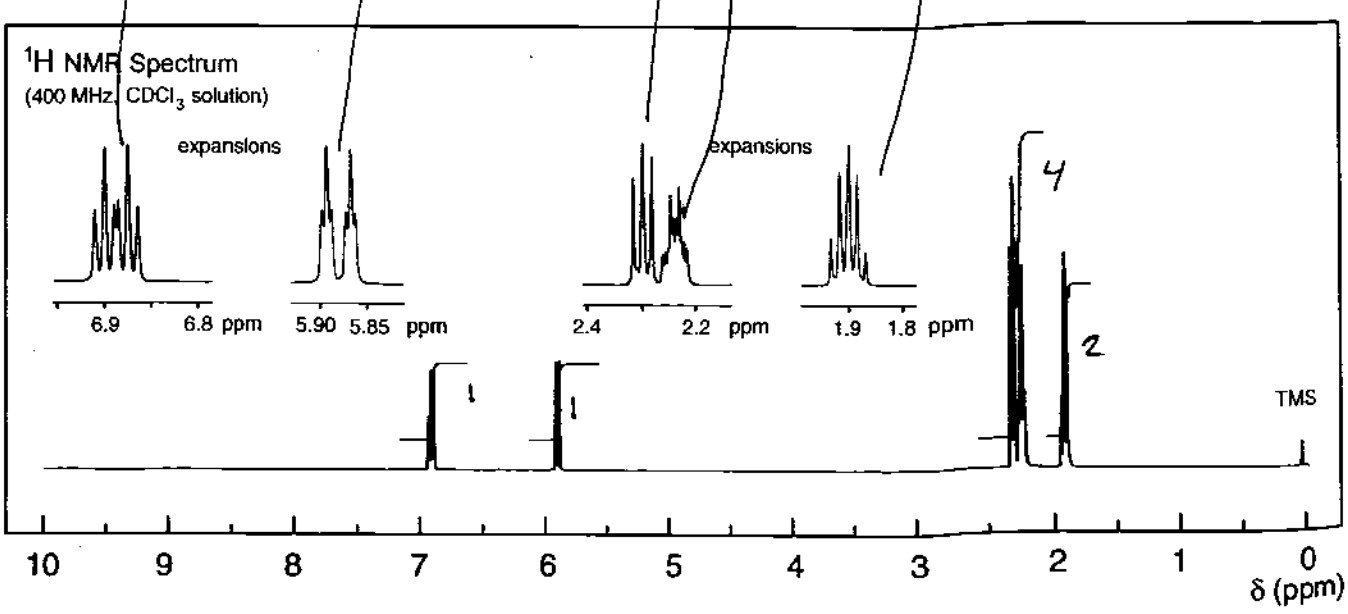
UV Spectrum

λ_{max} 225 nm ($\log_{10}\varepsilon$ 3.9)

solvent: methanol

6 - 4 + 1 = 3





8 OK, here's the doozy. I'm going to walk you through it a bit to help avoid panic.

* DON'T PANIC *

a) What obvious functional groups do you see on the first page?

-OH $C=C^{-H}$

b) Study the integration + the DEPT + tell me how many protons there are

16

c) How many unique carbon environments are there?

8

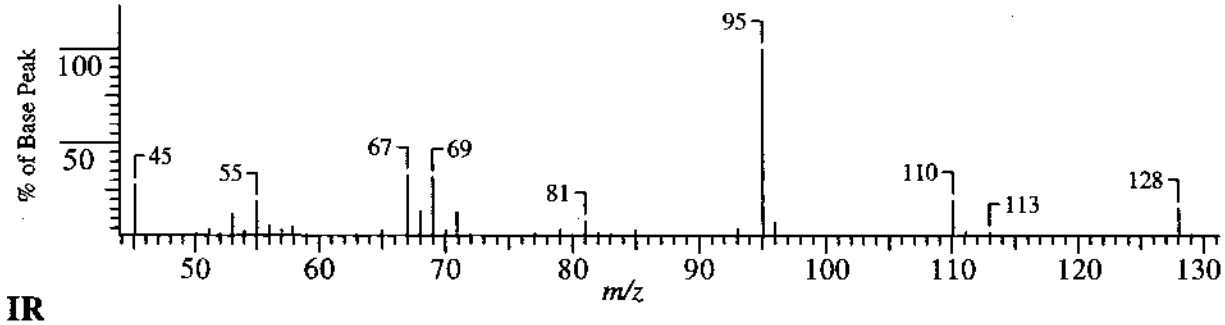
d) Now add up all that you had above + subtract it from the molecular ion mass.

$C_8H_{16}O = 128$ cha ching!

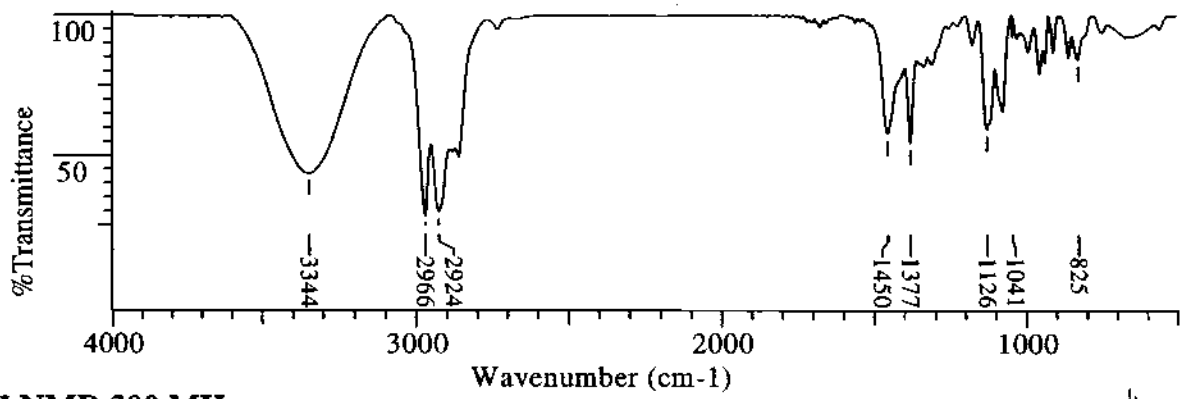
1 degree of unsaturation

Cont'd. L 2 pages

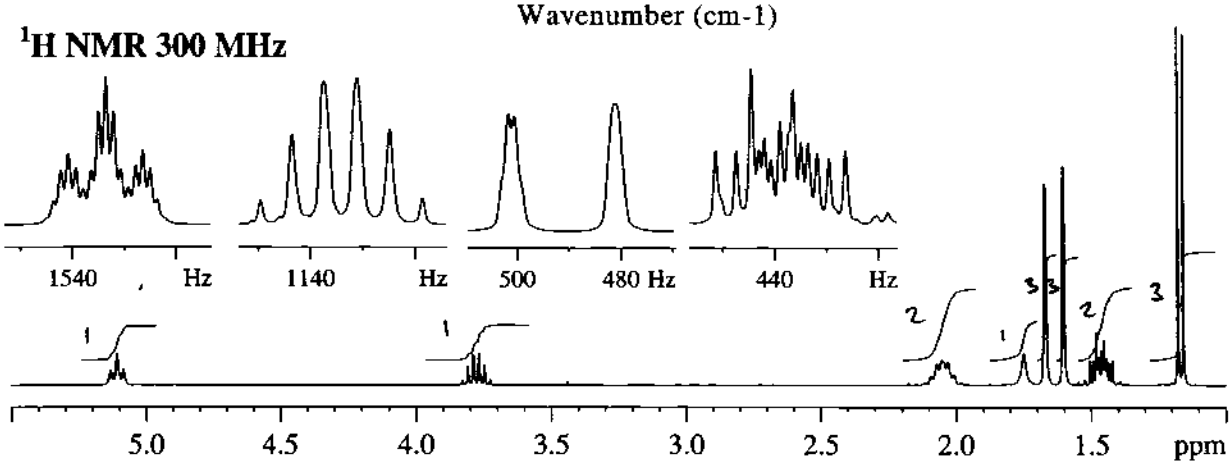
MASS



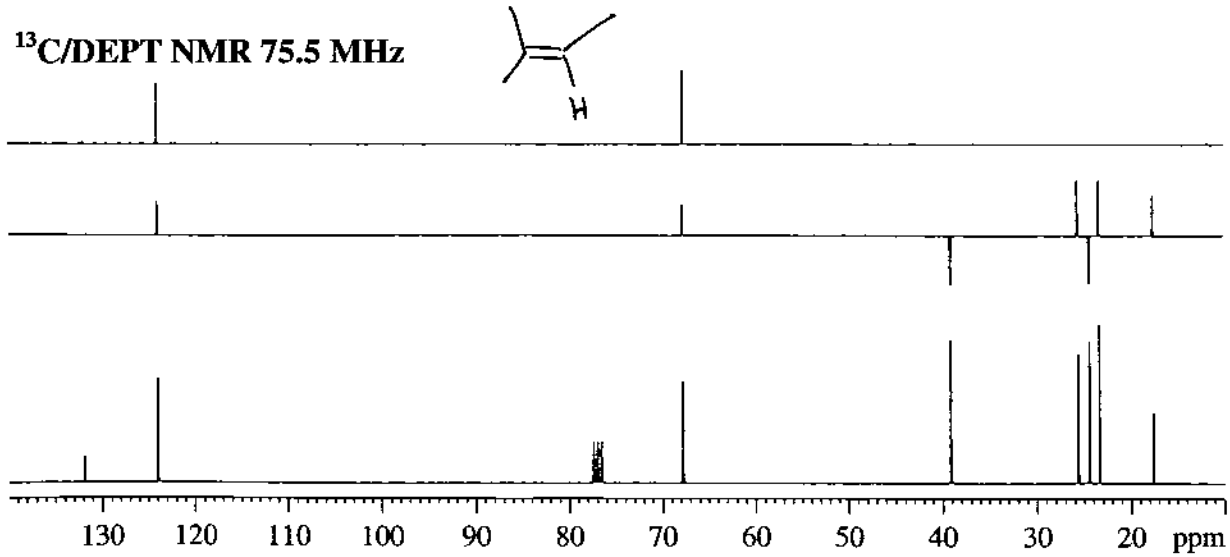
IR

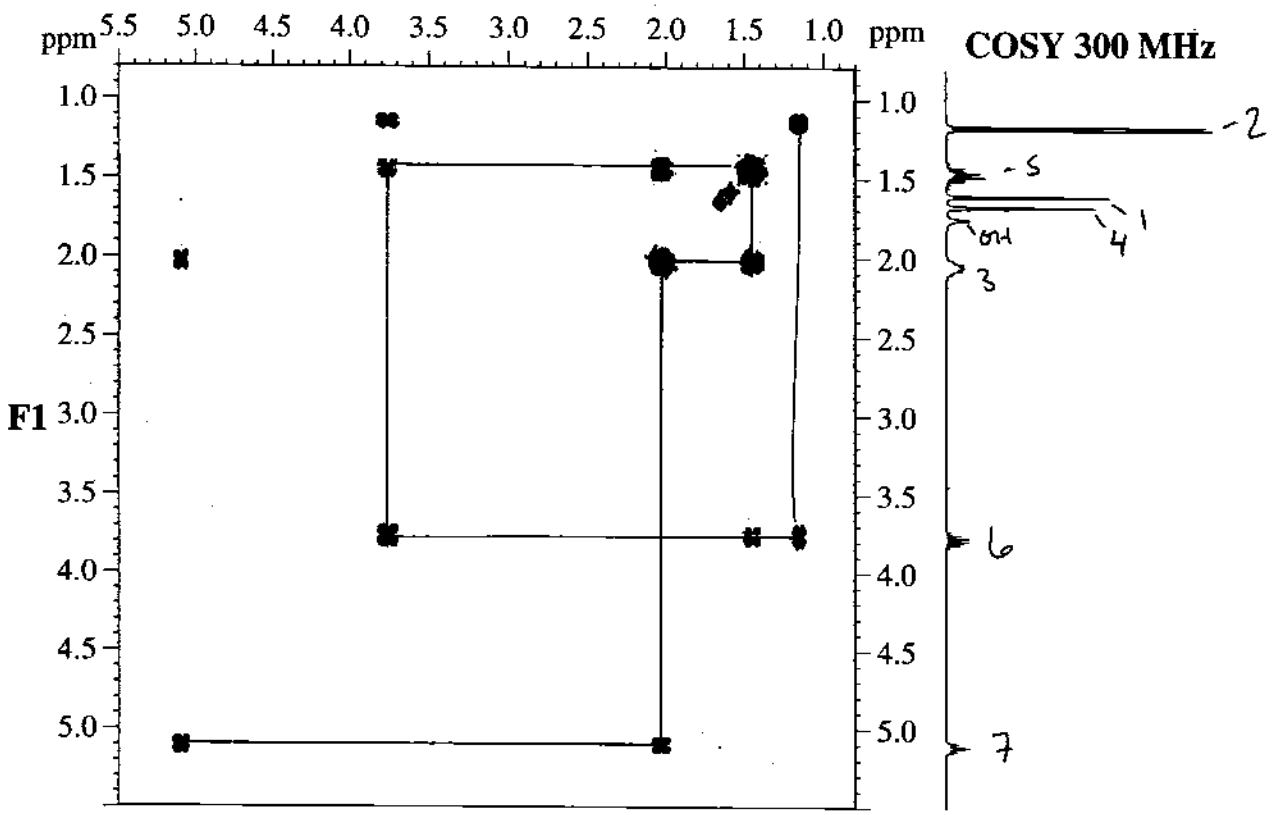


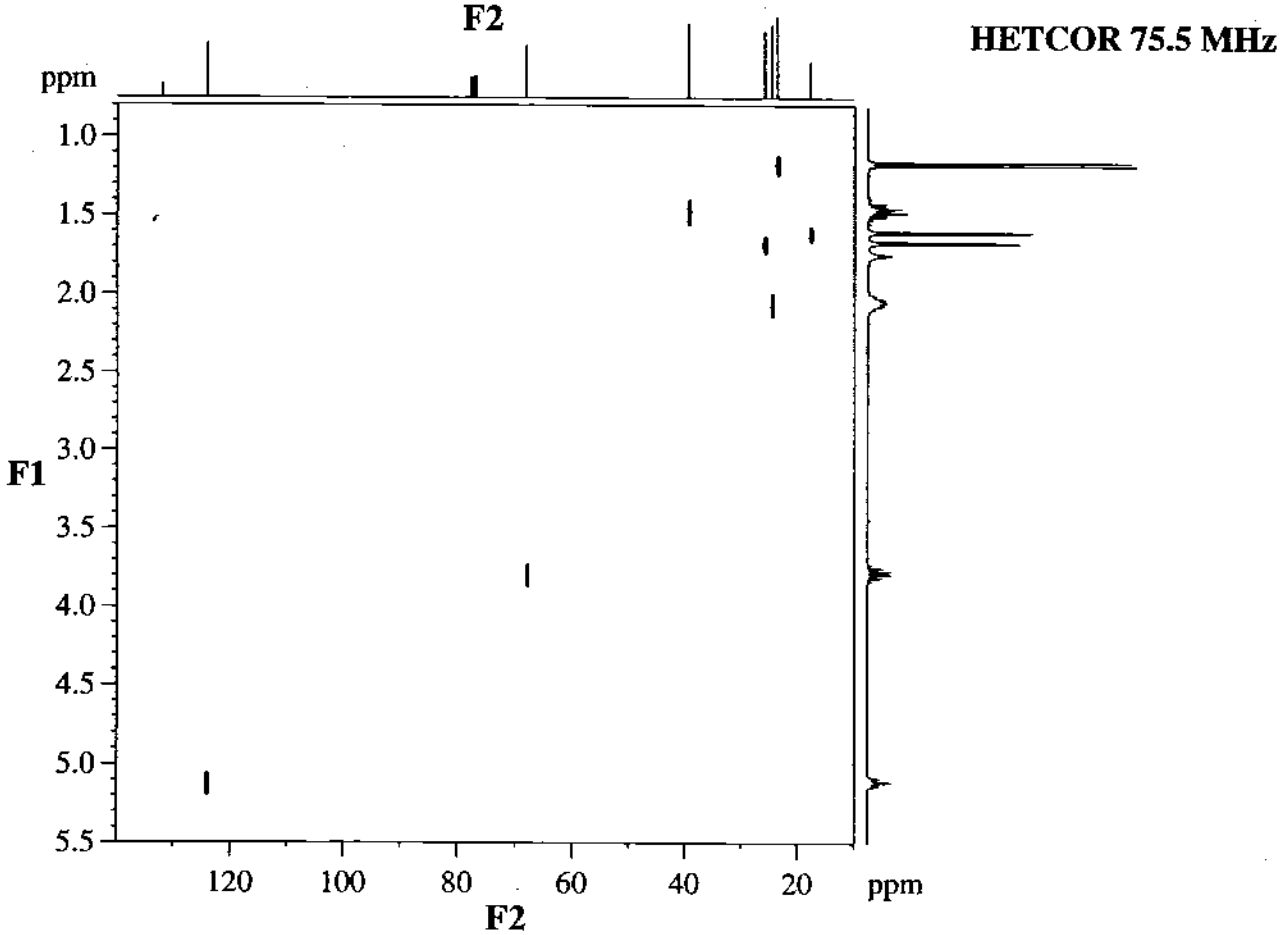
^{1}H NMR 300 MHz



^{13}C/DEPT NMR 75.5 MHz




COSY 300 MHz
ppm
5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
F1
F2
2
5
1
4
OH
3
6
7


HETCOR 75.5 MHz
ppm
F1
F2
120 100 80 60 40 20

e) 2D stuff.

Fill out the chart

	^{13}C	Mult	^{1}H	COSY correlations	Notes
1	18	CH_3	1.6, ~~●~~ brs		
2	23	CH_3	1.2, d	6	
3	24.2	CH_2	2.08, m	7, 5	
4	25.8	CH_3	1.7 s		
5	39	CH_2	1.5, m	3, 6	
6	68	CH	3.8, 6-et	2	
7	124	CH	5.15, dq	3	
8	132	C	na		

f) OK, what is it?