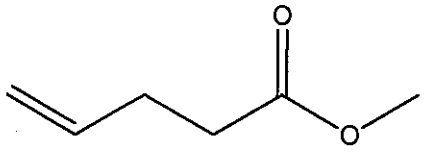
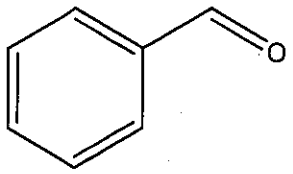
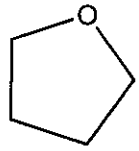
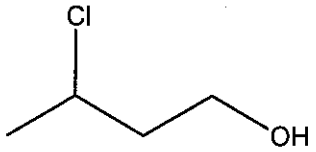
Handout 5: Proton NMR

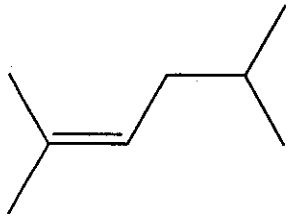
1. For the following molecules, mark each set of equivalent protons, then give an approximate chemical shift for that signal.

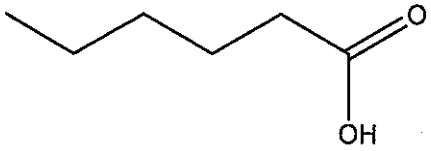


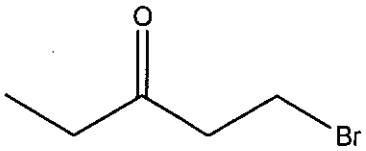




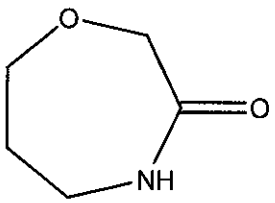


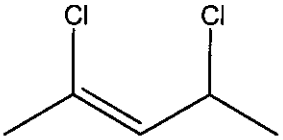


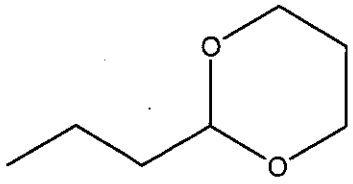


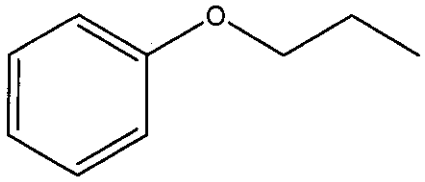


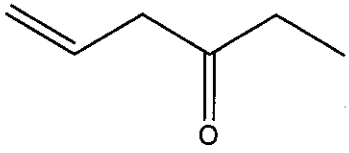
2. Do the same as problem 1, but consider any additive effects.







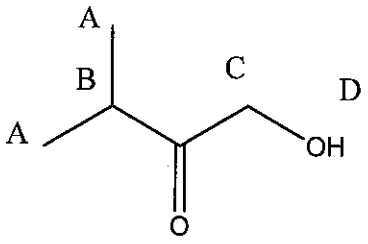




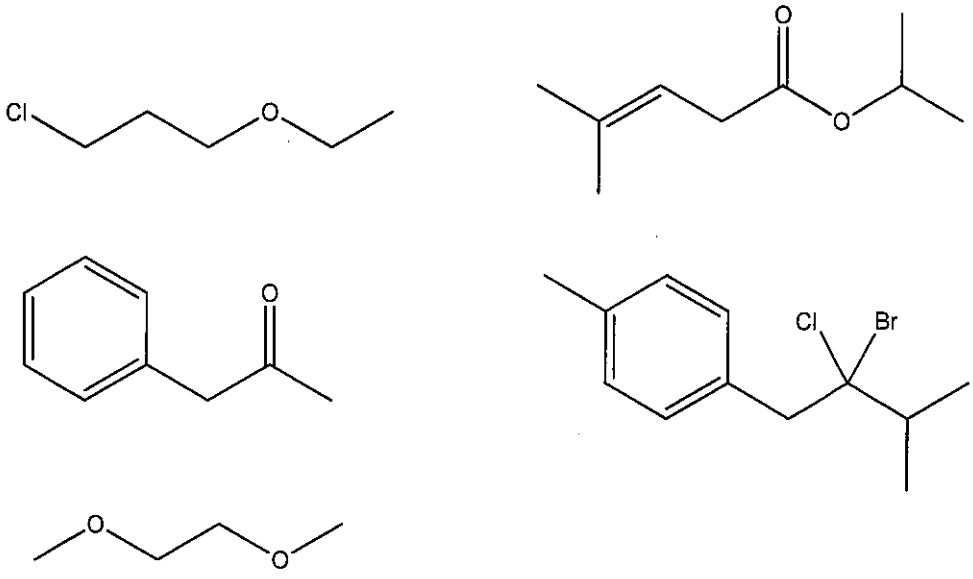
3. No matter how many sets of equivalent protons an aromatic ring has, we treat it as _____signal in proton NMR.

4. What is an exchangeable proton?

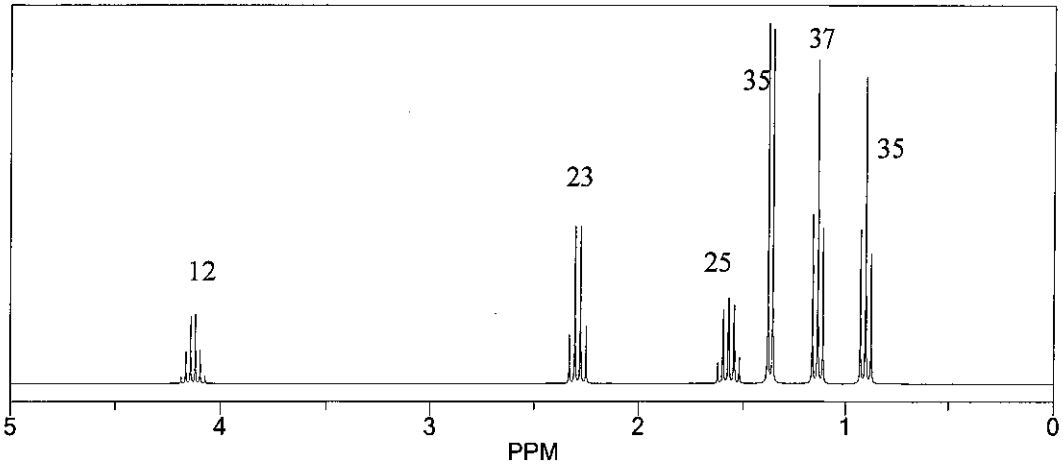
5. For the compounds below, indicate sets of equivalent protons. For each set, give its integration and multiplicity. Example:



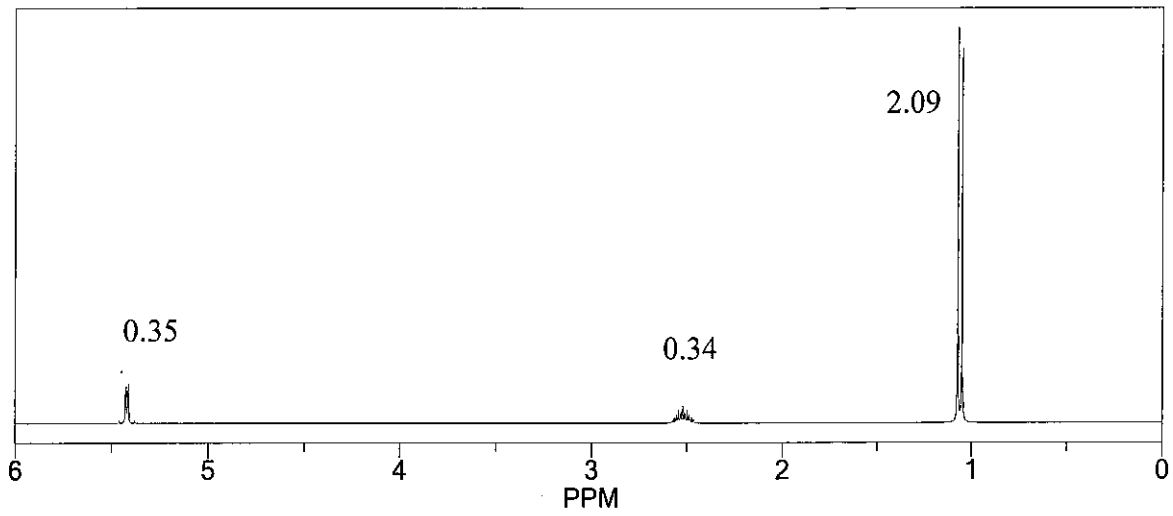
A; 6H, doublet
B: 1H, septet
C: 2H, singlet
D: 1H, singlet



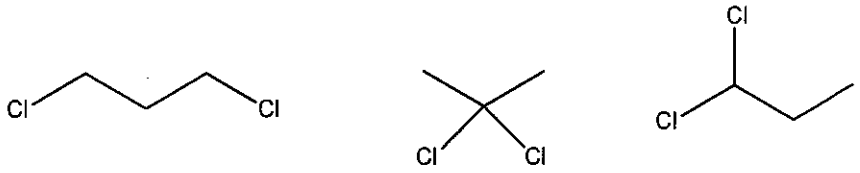
6. How many protons are represented by each signal in this spectrum of a $C_7H_{14}O_2$ compound?



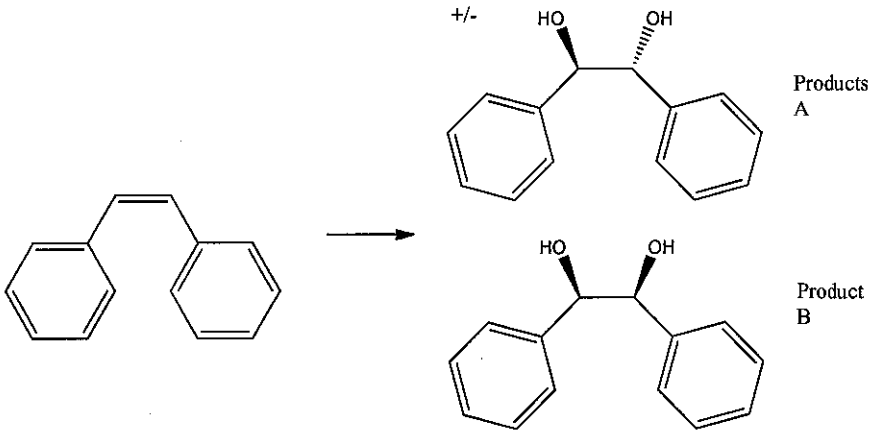
7. How many protons are represented by each signal in this spectrum of a C_8H_{16} compound?



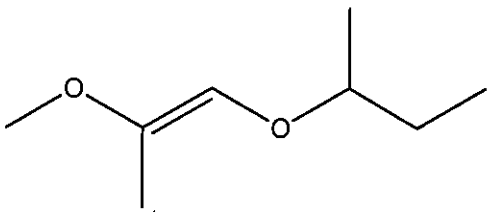
8. Draw the predicted proton and carbon spectra for these isomers. Can they be distinguished by NMR?

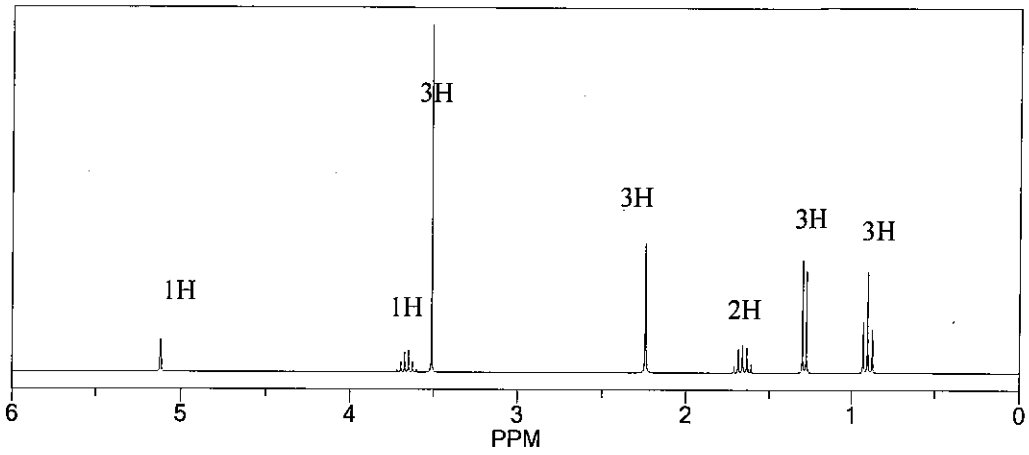


9. A dihyroxylation reaction of this alkene could potentially lead to either a racemic mix (A) or a meso product (B.) Can NMR be used to distinguish between these outcomes? Draw predicted proton and carbon NMR for both A and B as part of your answer.

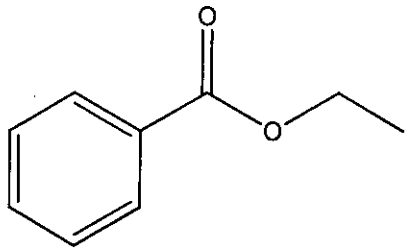


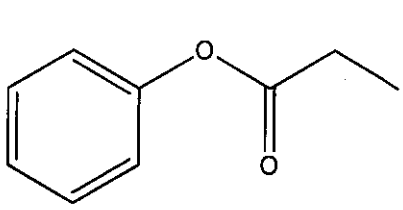
10. Is the proton NMR spectrum below consistent with this structure? Why or why not?

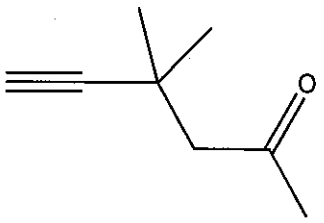


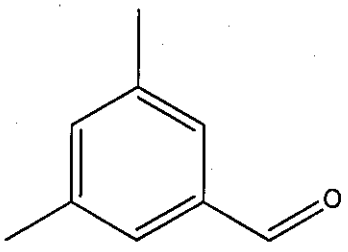


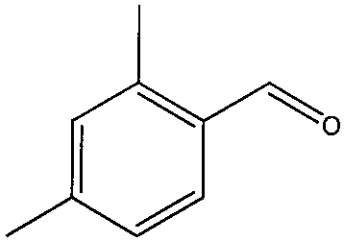
11. Draw predicted proton NMR spectra for these compounds.

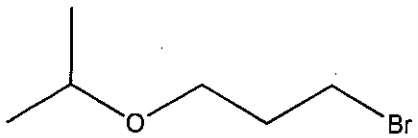






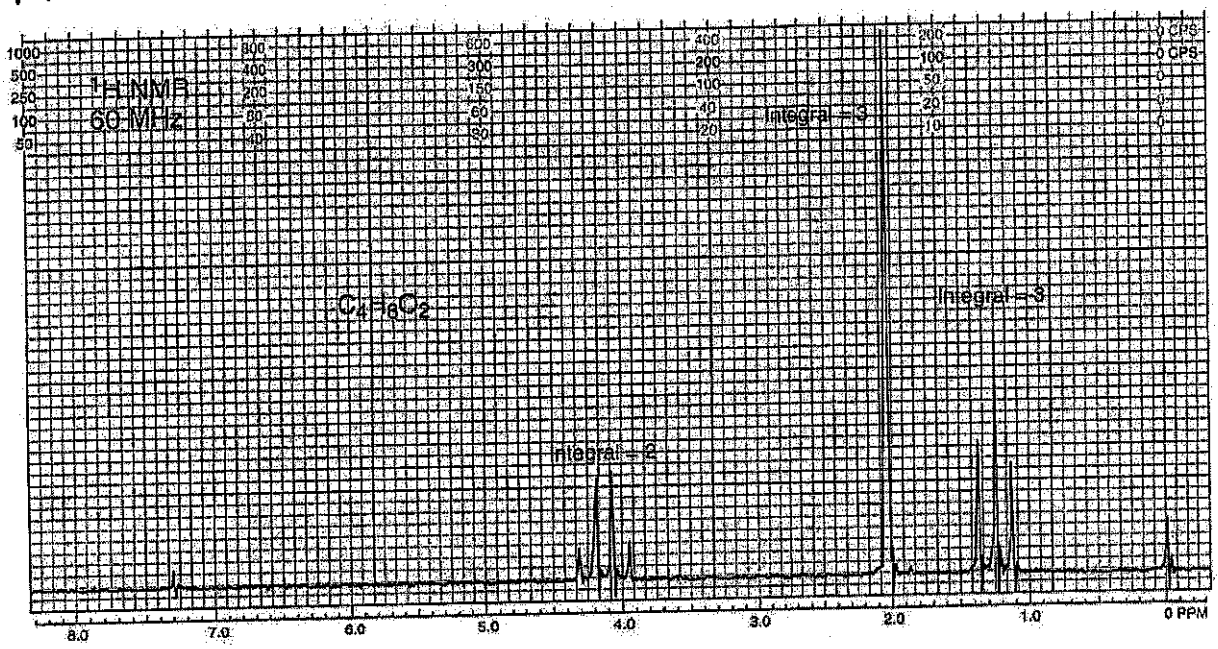




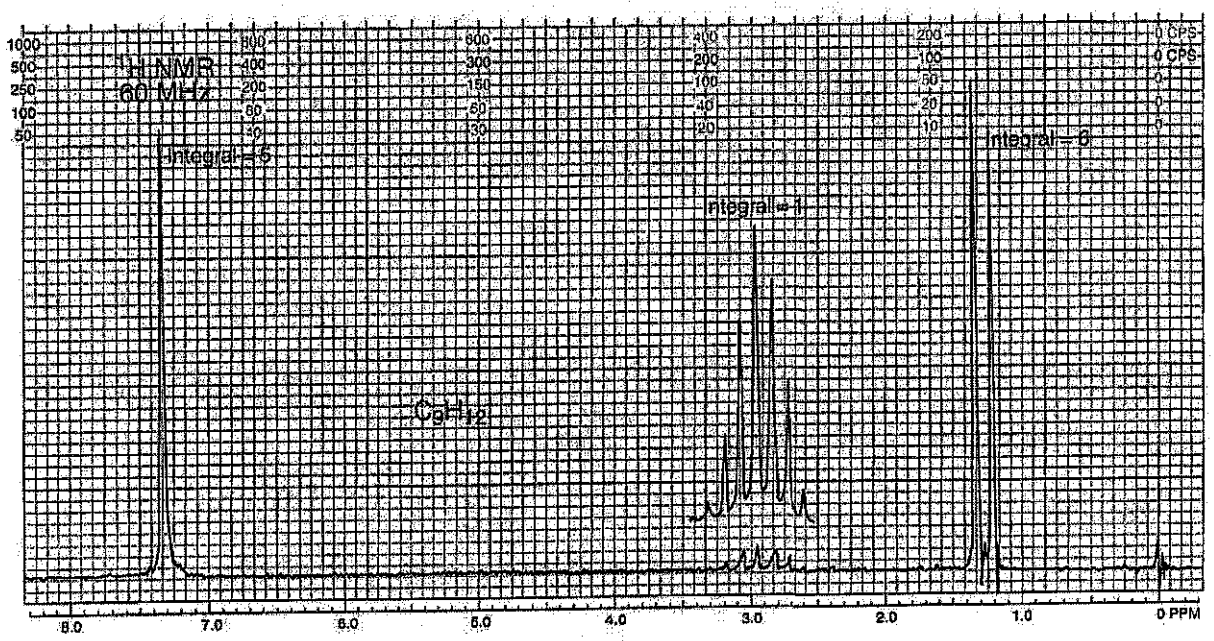


Proton NMR Problems

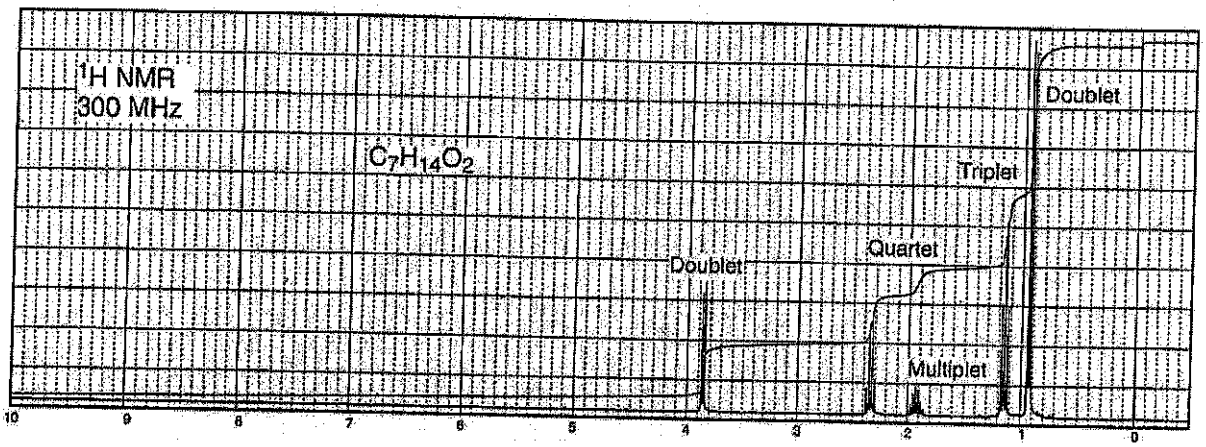
12. An ester



13. Aromatic Hydrocarbon

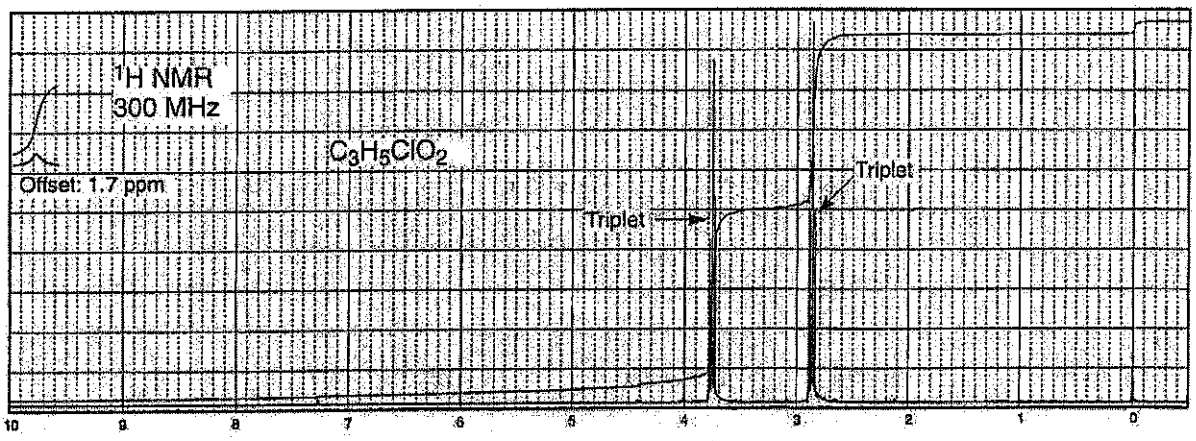


14 An ester



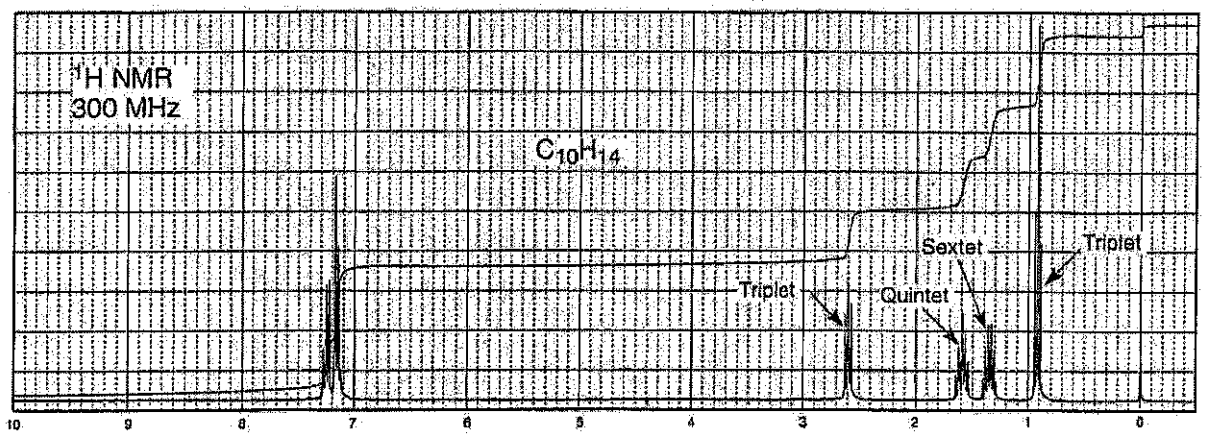
Integral 2 2 1 3 6

15 A carboxylic acid



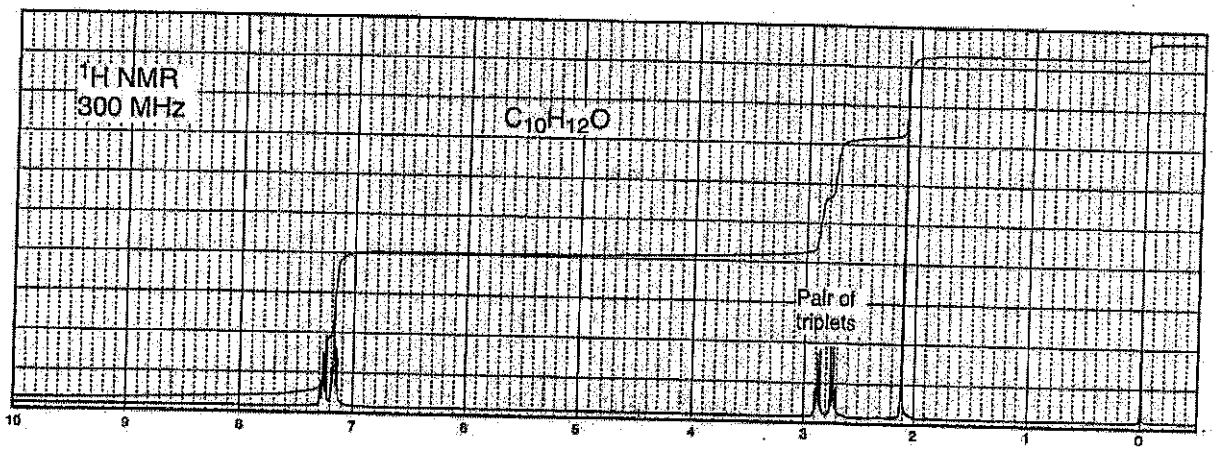
Integral 1 2 2

16 A hydrocarbon



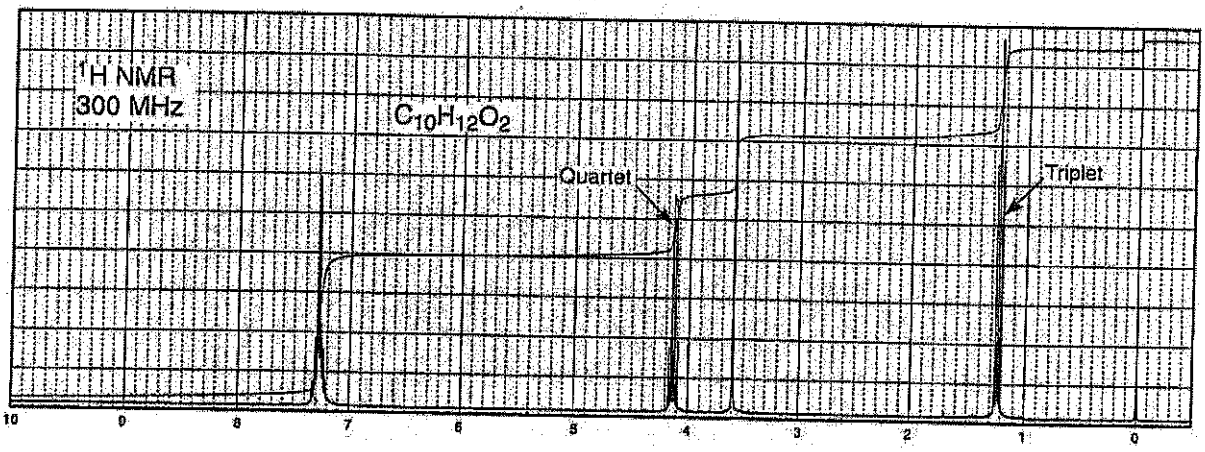
Integral 5 2 2 3

17 A ketone



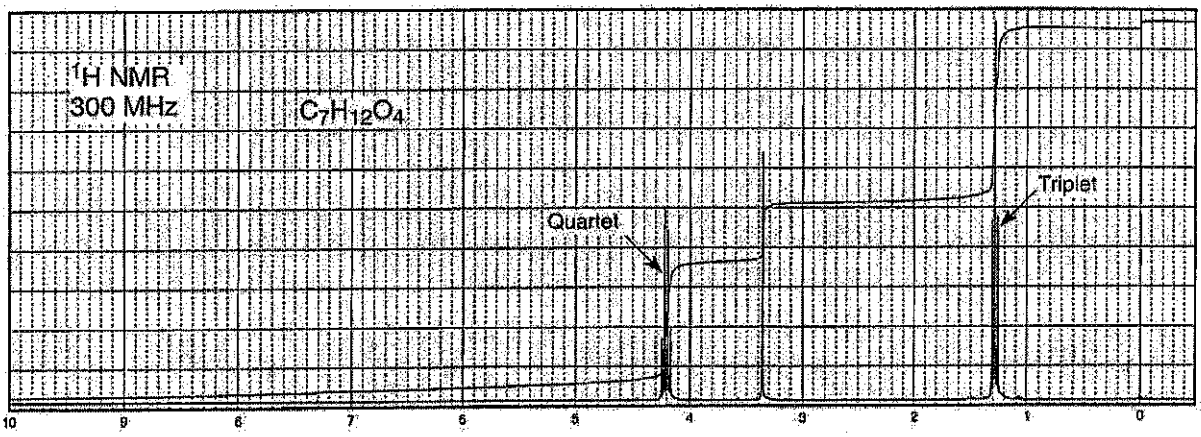
Integral 5 2 2 3

18 An ester



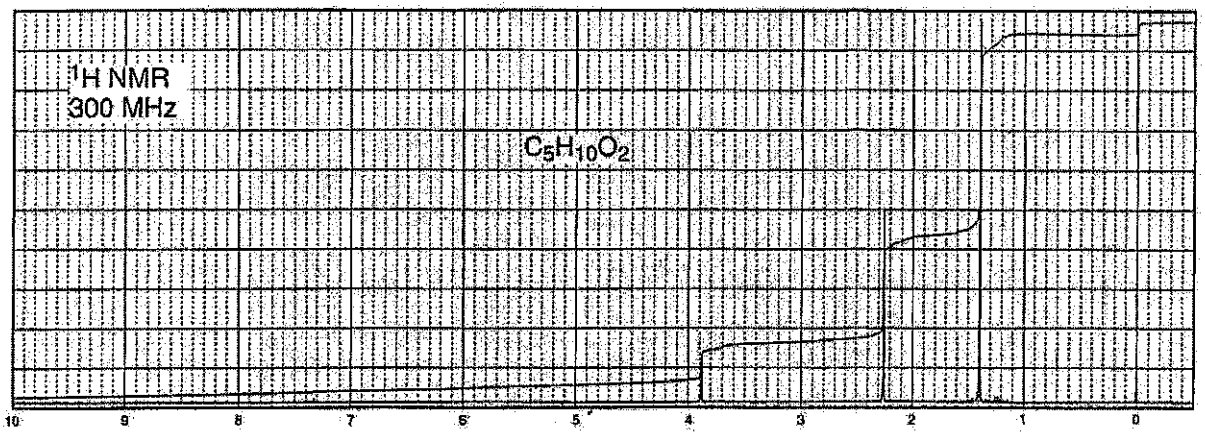
Integral 5 2 2 3

19. An ester



Integral Height: 3.1 1.5 4.4

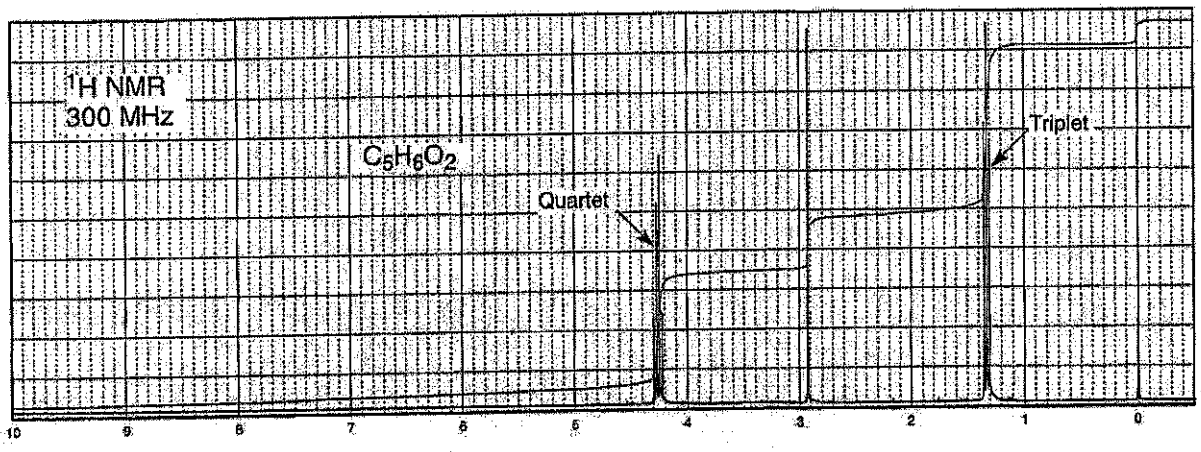
20. Characteristic IR peaks: 3450 cm^{-1} (broad, smooth); 1713 cm^{-1} (intense)



Integral 1 3 6

→ one exchangeable proton

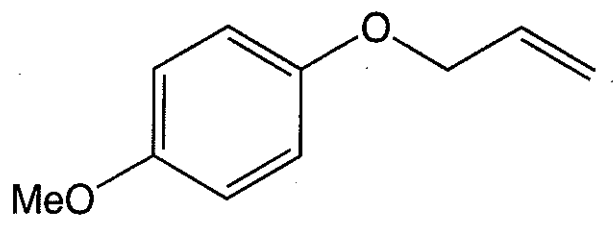
21. Characteristic IR peaks: 3270 cm^{-1} (medium); 2118 cm^{-1} (medium sharp), 1727 cm^{-1} (intense)



Integral 2 1 3

22. The proton NMR below is for allyloxyanisole (shown below). Expansions are shown for each of the five unique types of protons other than the aromatic protons (which you can ignore) and the OMe at 3.78 ppm. Hertz values are given for each peak.

a) Describe each multiplet in terms of doublet, triplet, etc. in the spaces provided.
b) Determine all coupling constants for each multiplet and label them appropriately (i.e. J_{ab}, J_{cd}, etc.).
c) Assign the protons directly on the structure below using the letters a, b, c, and d.

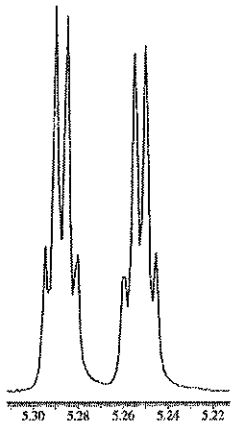


Ha

peaks (Hz)
1350.13
1348.66
1347.18
1344.98
1343.51
1342.04

multiplet? _____

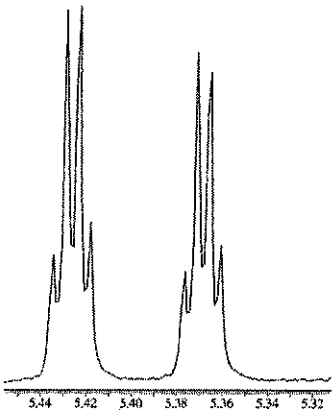
Hb



peaks (Hz)
1589.12
1587.65
1586.18
1584.71
1578.46
1577.35
1575.88
1574.41

multiplet? _____

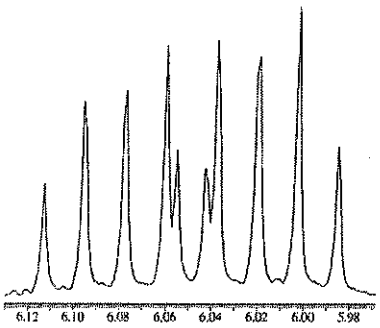
Hc



peaks (Hz)
1631.04
1629.57
1627.73
1626.26
1613.75
1612.28
1610.45
1608.97

multiplet? _____

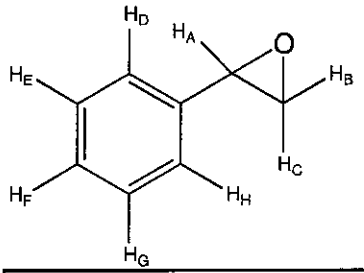
Hd

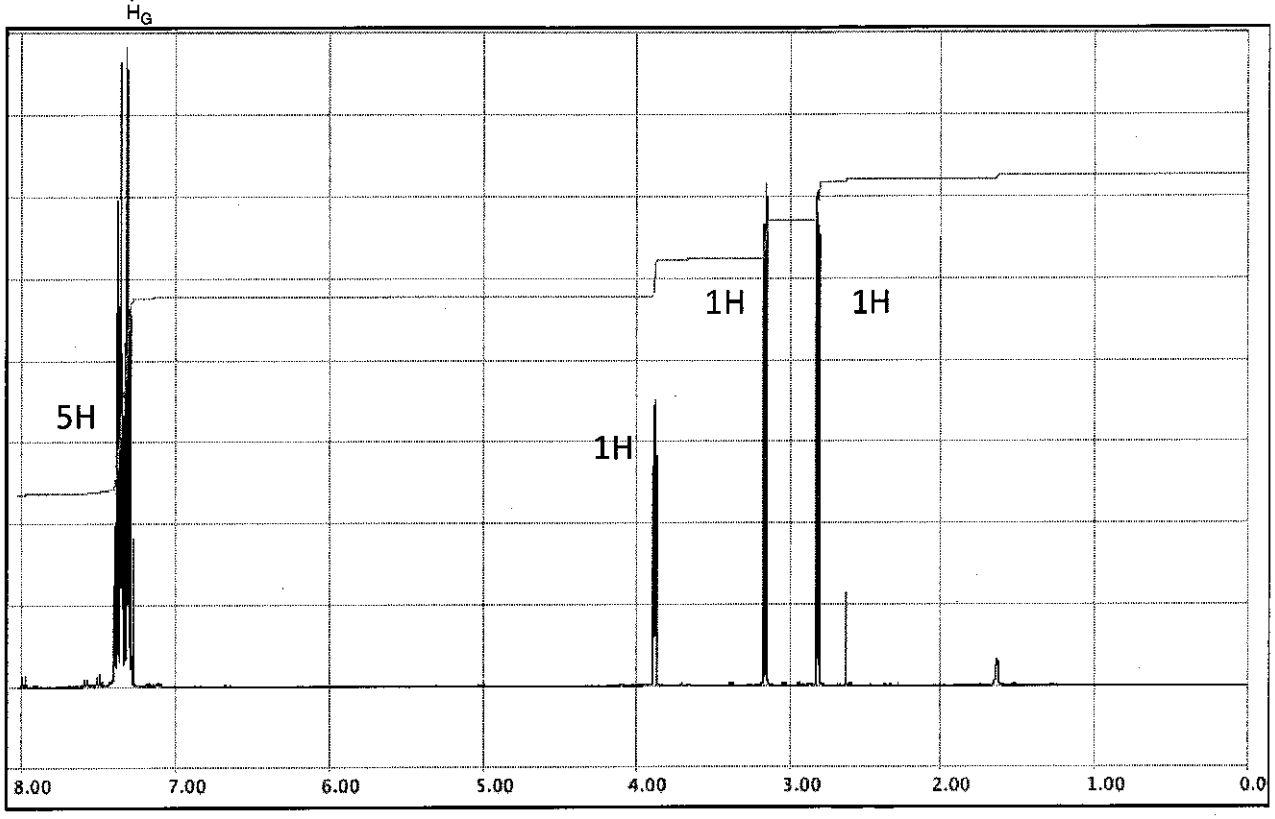


peaks (Hz)
1834.73
1829.58
1824.07
1818.92
1817.45
1813.77
1812.30
1806.79
1801.64
1796.49

multiplet? _____

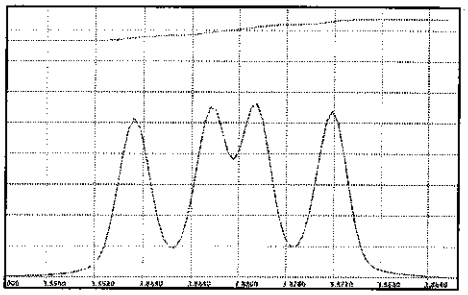
23. Below is the ^{1}H NMR spectrum of epoxystyrene:





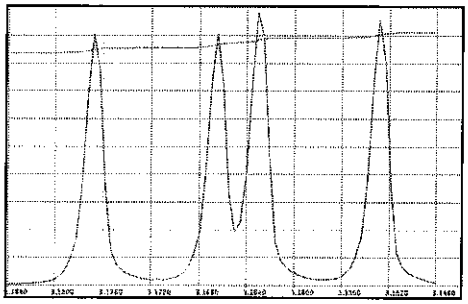
a) Assign peaks for protons H_A, H_B, and H_C. (Label the peaks directly on the spectrum).

b) Given the ppm values shown in the expansions on the next page, calculate all relevant coupling constants for H_A, H_B, and H_C, and analyze each multiplet that is shown on the next page. Use tree diagrams to show the splitting pattern in each case, and describe each one (doublet, triplet, quartet, doublet of doublets, doublet of triplets, etc.). You do not need to analyze the multiplet in the aromatic region.



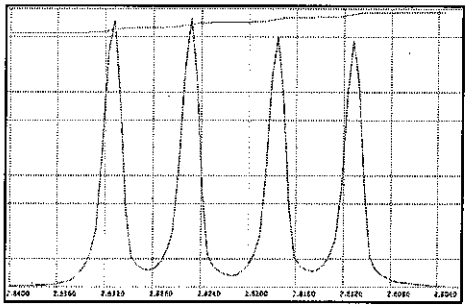
Peak data in Hz:

345.31
342.75
341.25
338.69



Peak data in Hz

282.00
277.94
276.50
272.44



Peak data in Hz

250.56
248.00
245.06
242.50