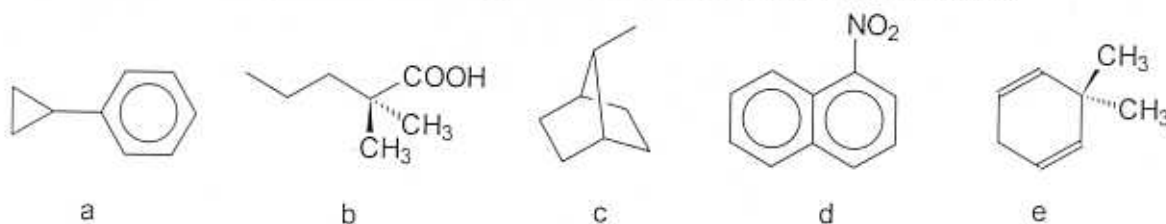


Chemistry 304, Problem Set 1

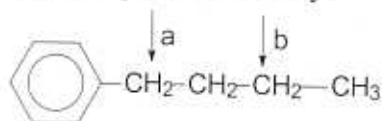
- Comment on the following statements:
 - Only nuclei with spin quantum numbers of $\frac{1}{2}$ can be observed by NMR
 - Chemical shifts, when expressed as δ values, are dimensionless
 - Coupling constants are expressed in units of cm^{-1}
 - Increased field strengths provide improved signal-to-noise ratios during NMR.
 - ^{13}C - ^{13}C coupling is not commonly observed (Why?)
- Predict the appearances of proton and ^{13}C NMR spectra for 1,3-dichlorobutane.

- How many non-equivalent kinds of protons do the following structures have?



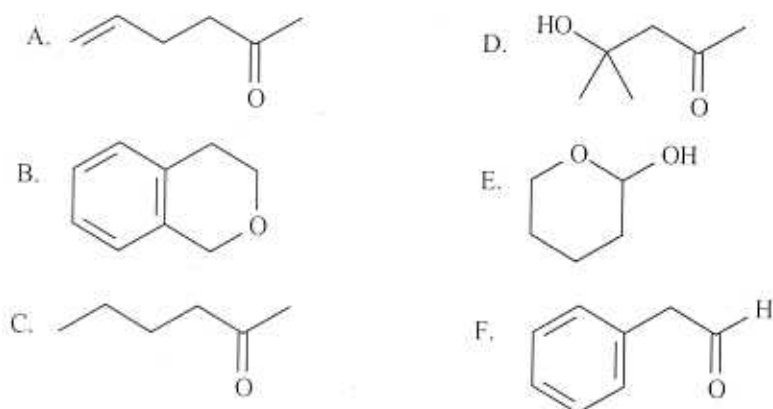
- Using 1-bromo-2-chloroethane as example, explain the $n+1$ rule of multiplicity and predict the relative appearance of a proton NMR spectrum of this compound!

- The protons a in n-butylbenzene shown below have a significantly different chemical shift from the protons b. Why?

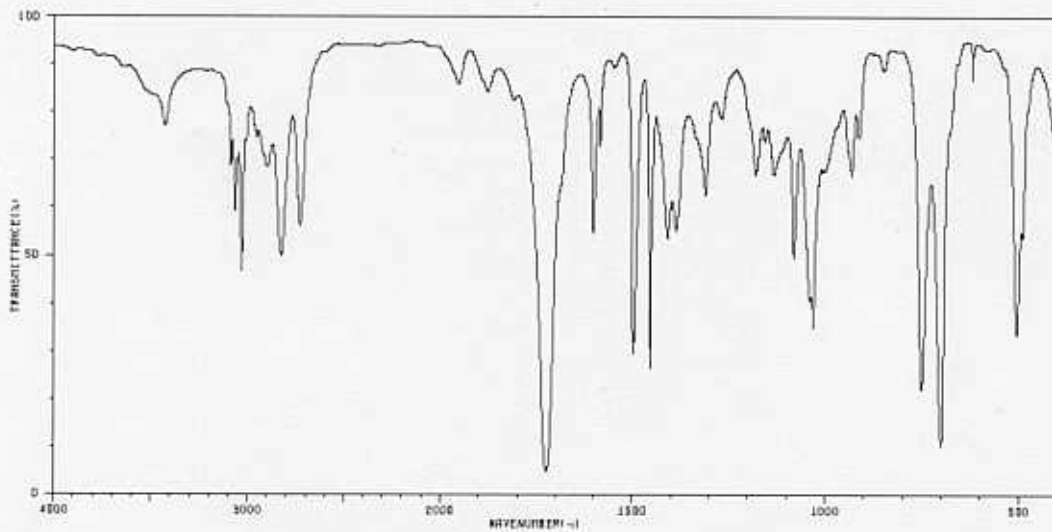


- Show structural formulas for all isomeric alcohols $\text{C}_4\text{H}_{10}\text{O}$ and predict the number of signals for their decoupled ^{13}C NMR spectra.

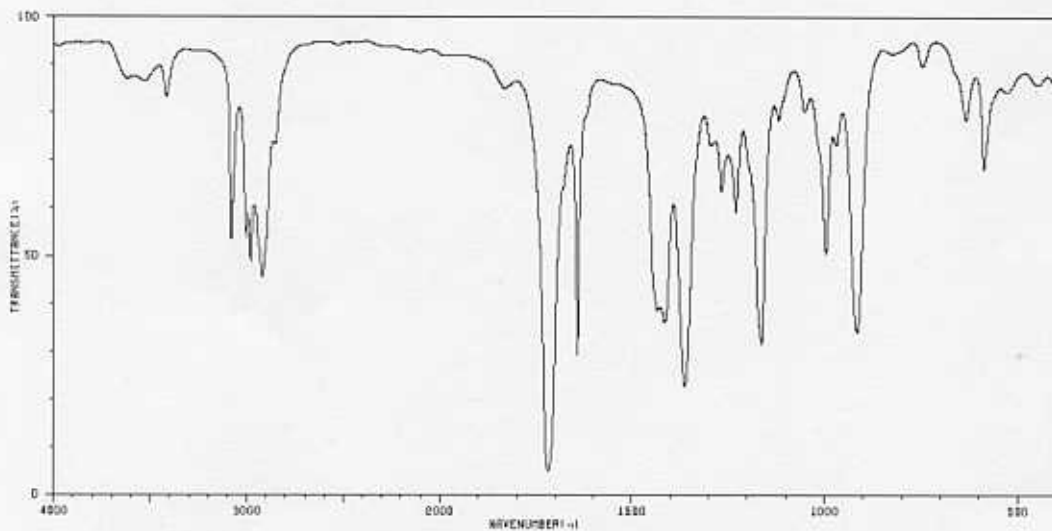
MATCH a structure from the list below to the following IR spectra. Place the letter of the structure in the blank to the left of the spectrum.



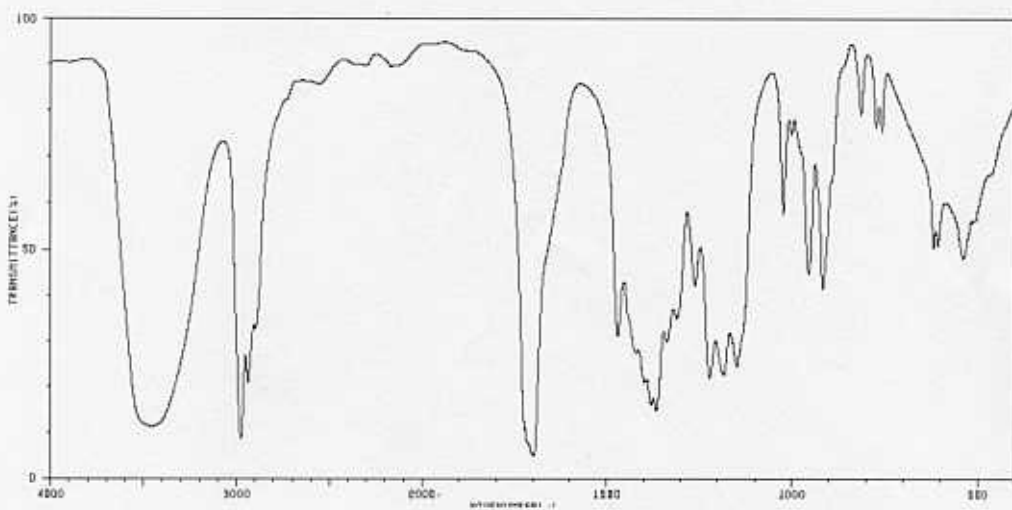
a)



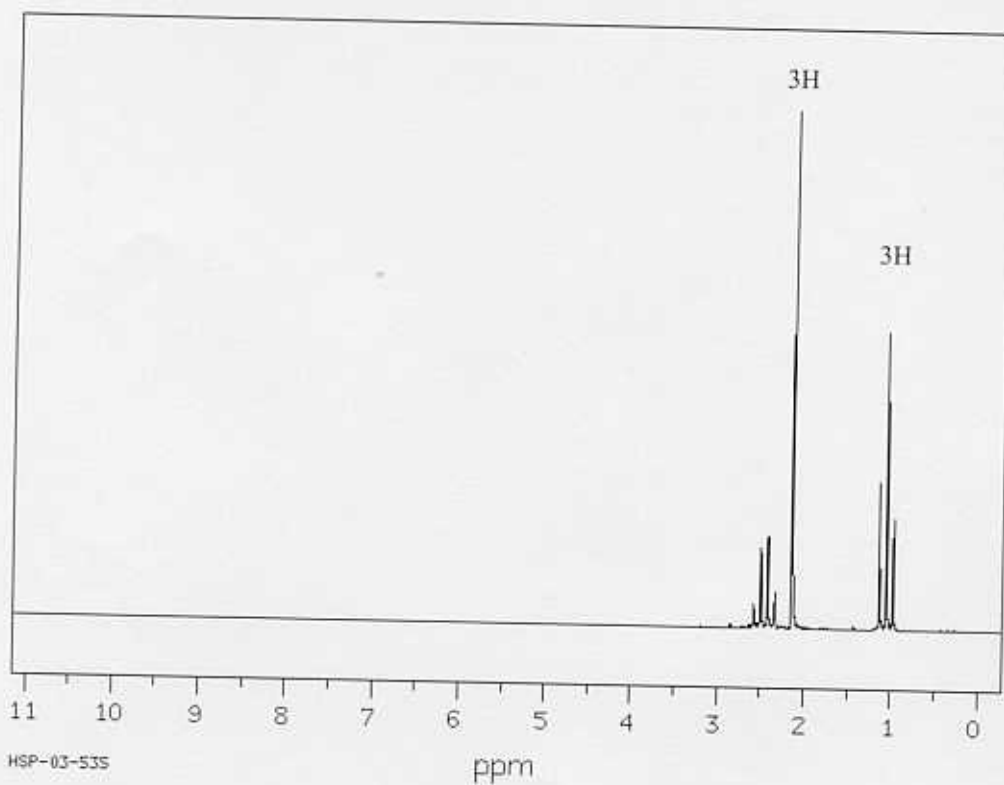
b)



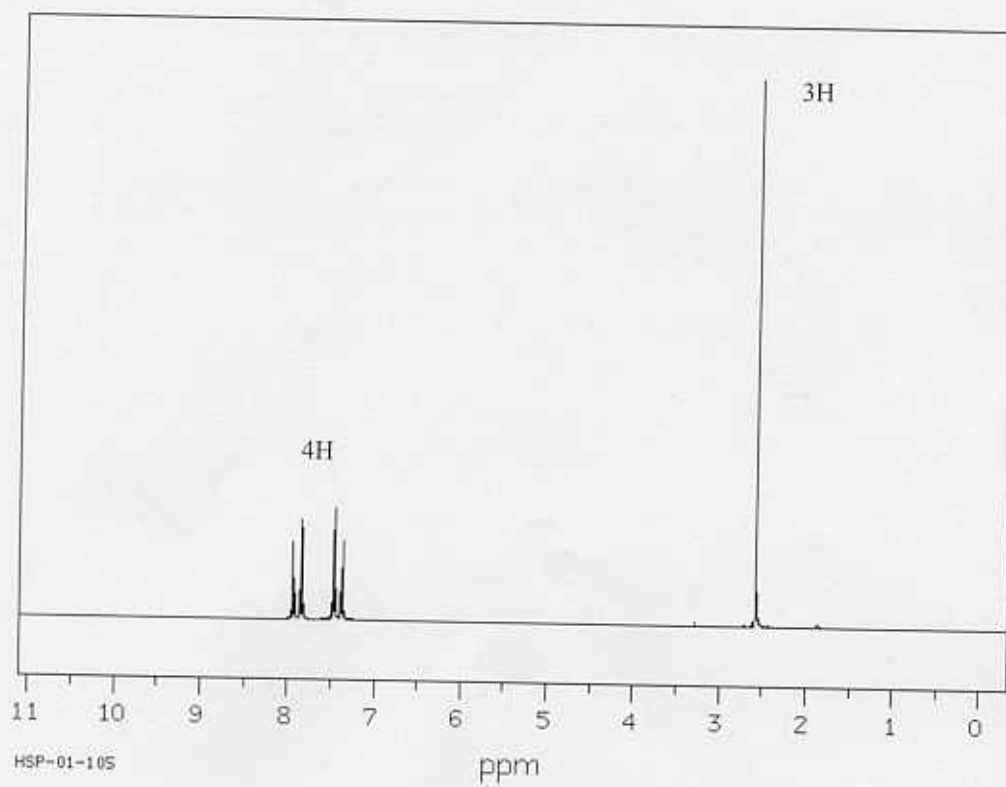
c)



7. Suggest a structure for the compound, C_4H_8O , the proton NMR spectrum of which is shown below:



8. Suggest a structure for the ketone, C_8H_7ClO , the proton NMR spectrum of which is shown below:

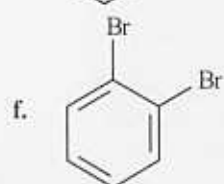
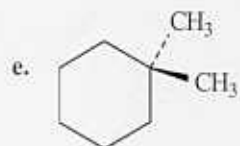
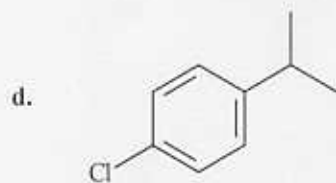
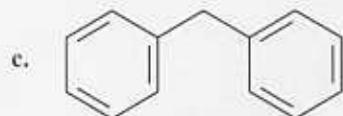
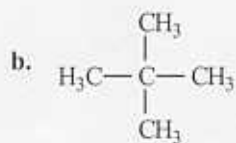


9. The following questions pertain to the charting of NMR spectra. MATCH a term to each description below. Place the letter of the term in the blank to the left of the description.

- a. TMS
- b. high-field or upfield side
- c. MHz
- d. delta (δ)
- e. low-field or downfield side
- f. chemical shift
- g. specific absorption

- A. ____ When looking at an NMR chart the right-hand part of the chart is the ____.
- B. ____ The exact place on the chart at which a nucleus absorbs is called its ____.
- C. ____ The calibration standard for ^1H and ^{13}C NMR is:
- D. ____ The NMR charts are calibrated using an arbitrary scale that is divided into ____ units.

10. For each of the compounds below tell how many signals you would expect the molecule to have in its normal, broadband decoupled ^{13}C NMR spectra.



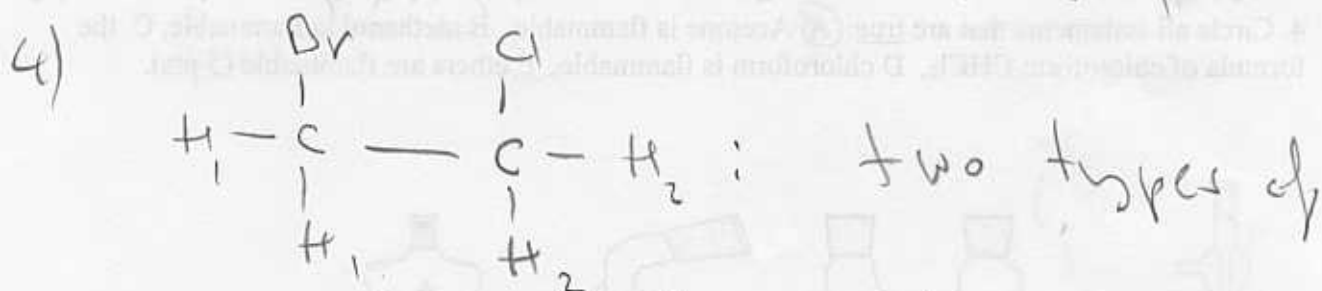
304 Prob 1 Key

1) a false b true c false
 d true e it is not probable
 to find two ^{13}C 's
 side-by-side

2) ^{13}C : four signals

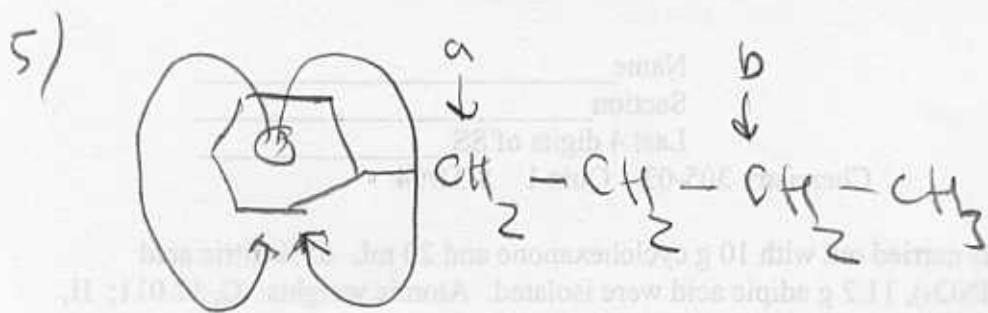
^1H : triplet, 2H
 quartet, 2H
 sextet, 1H
 doublet, 3H

3) a-6 b-5 c-7 d-7 e-4

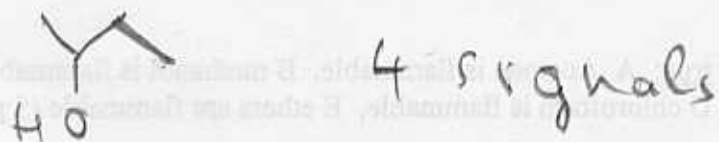
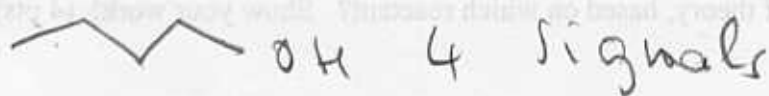
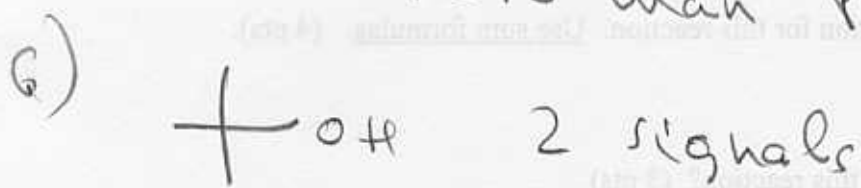


equivalent protons. Consider
 type 1: their signal is split
 because of the following spin align-
 ments for protons 2:

$\begin{array}{ccc} \uparrow\uparrow & \uparrow\downarrow & \downarrow\downarrow \\ \downarrow\downarrow & & \end{array}$
 so we observe a triplet
 for protons 1.



The ring current of the benzene ring deshields protons a much more than protons b.

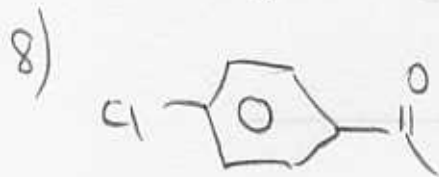
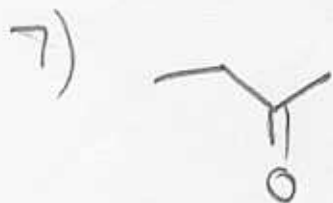


IR spectra:

a - F

b - A

c - D



9) A - b B - f C - a D - d

10) a - 3 b - 2 c - 5 d - 6
 e - 5 f - 3



2. What is the limiting reactant of this reaction? (2 pts)

3. What is the percent yield of theory, based on which reactant? Show your work. (4 pts)

4. Give the reactions that are true: A. Acetone is flammable. B. methanol is flammable. C. the formula of carbon monoxide is CH₂. D. chloroform is flammable. E. ethane is flammable. (3 pts)



5. Provide reasonable names for the objects shown above. (4 pts)

A _____
 B _____
 C _____
 D _____