

Chem 333, Exam 1
Professor Fox
FALL 2009

Your Name _____

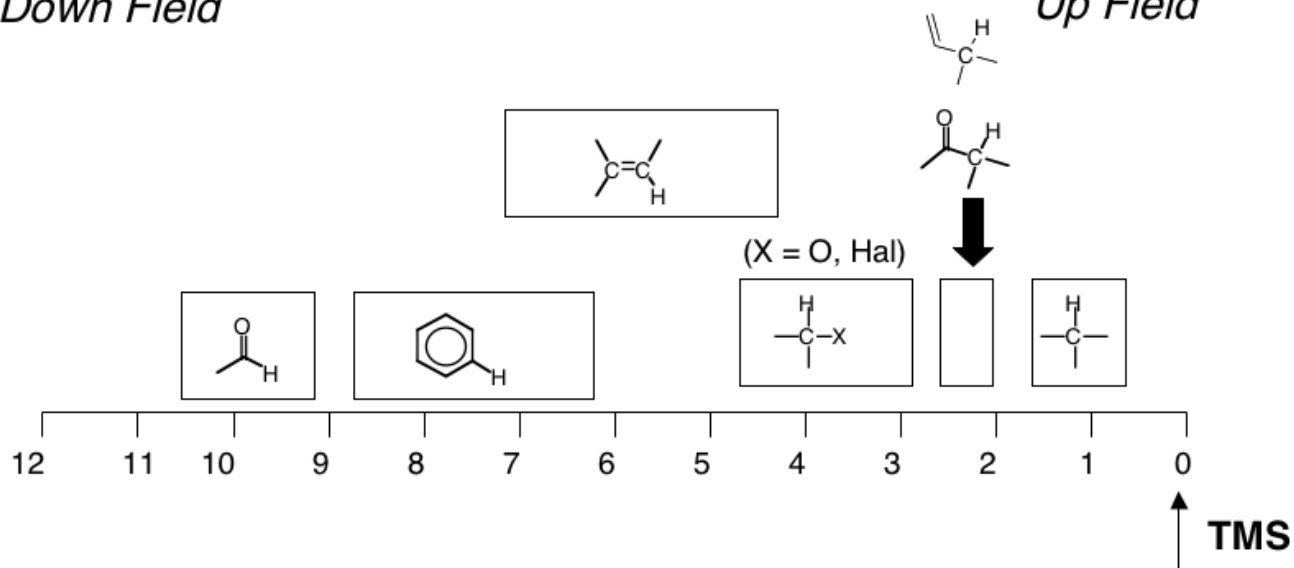
- 1) 9 points
- 2) 9 points
- 3) 12 points
- 4) 22 points
- 5) 48 points

Overview of typical ^1H NMR shifts

Note: alkene region modified from earlier handout

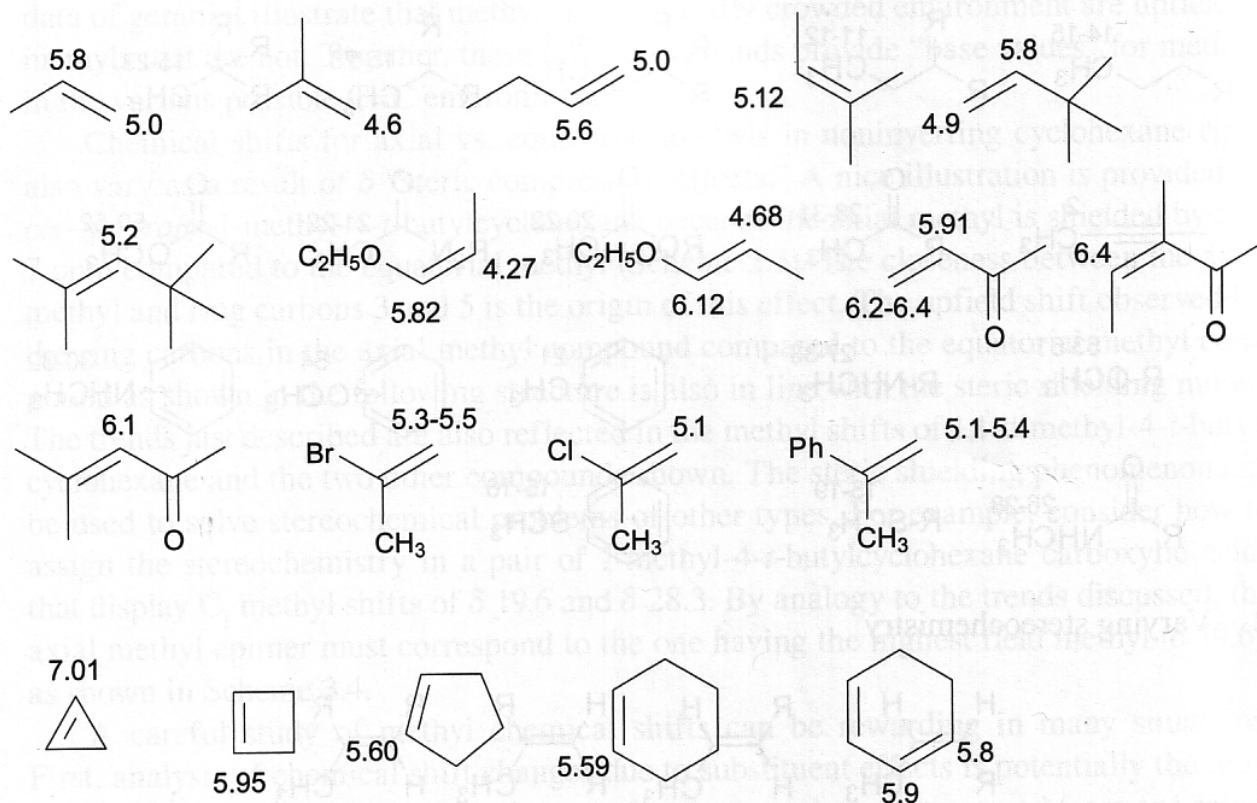
Down Field

Up Field



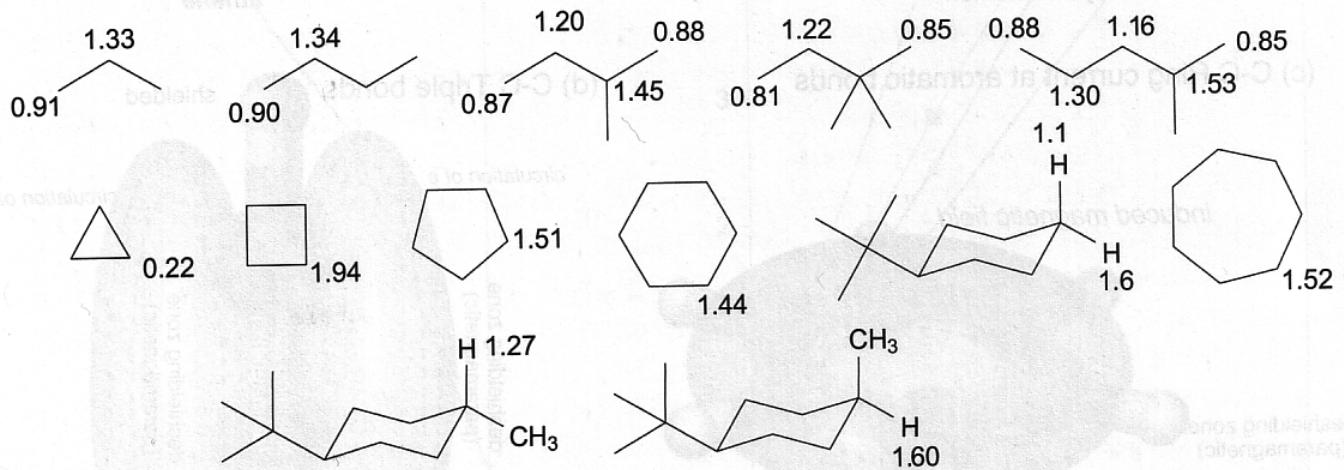
^1H NMR Tables

Experimental sp^2 ^1H chemical shifts (ppm).

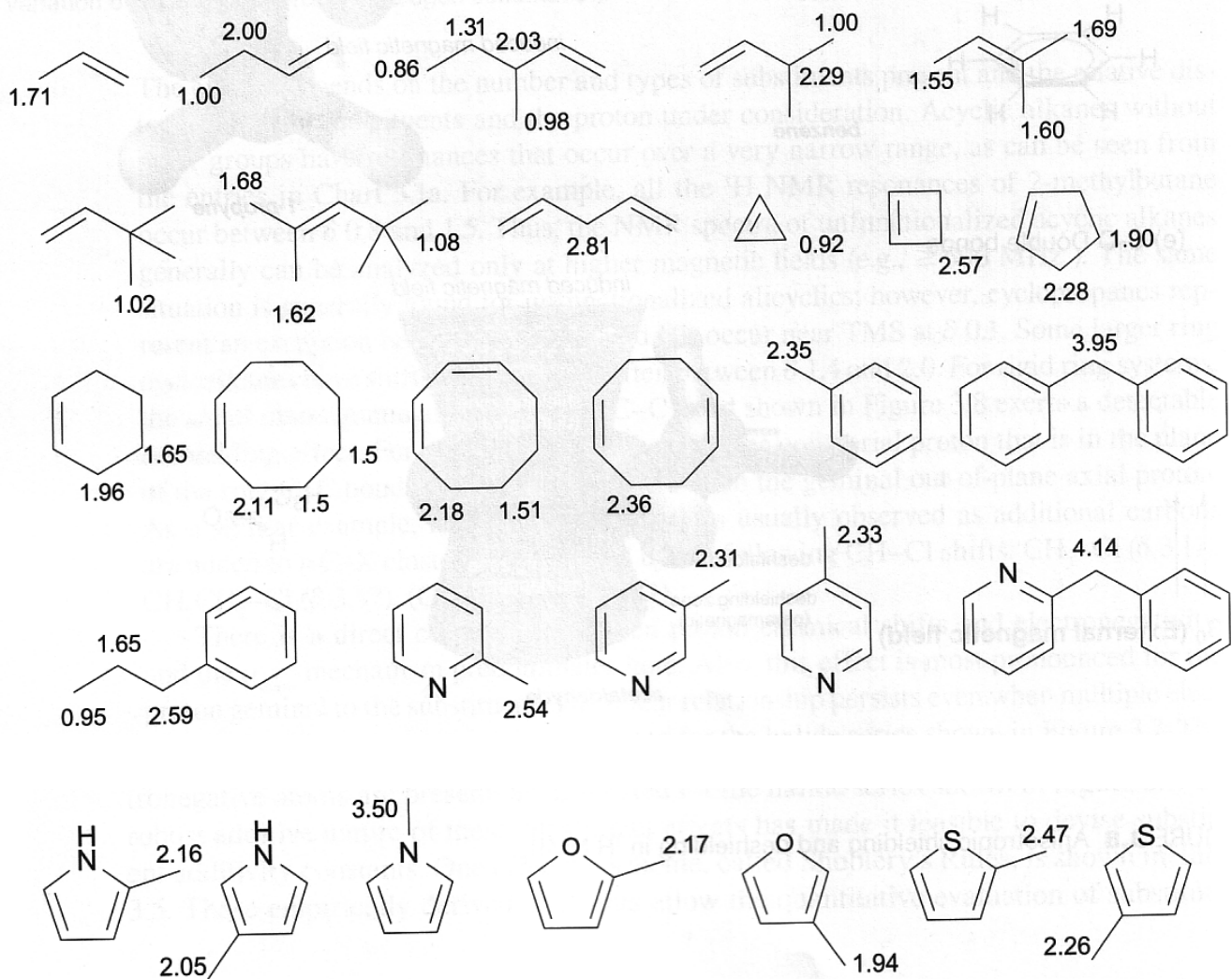


^1H NMR Tables

Alkanes



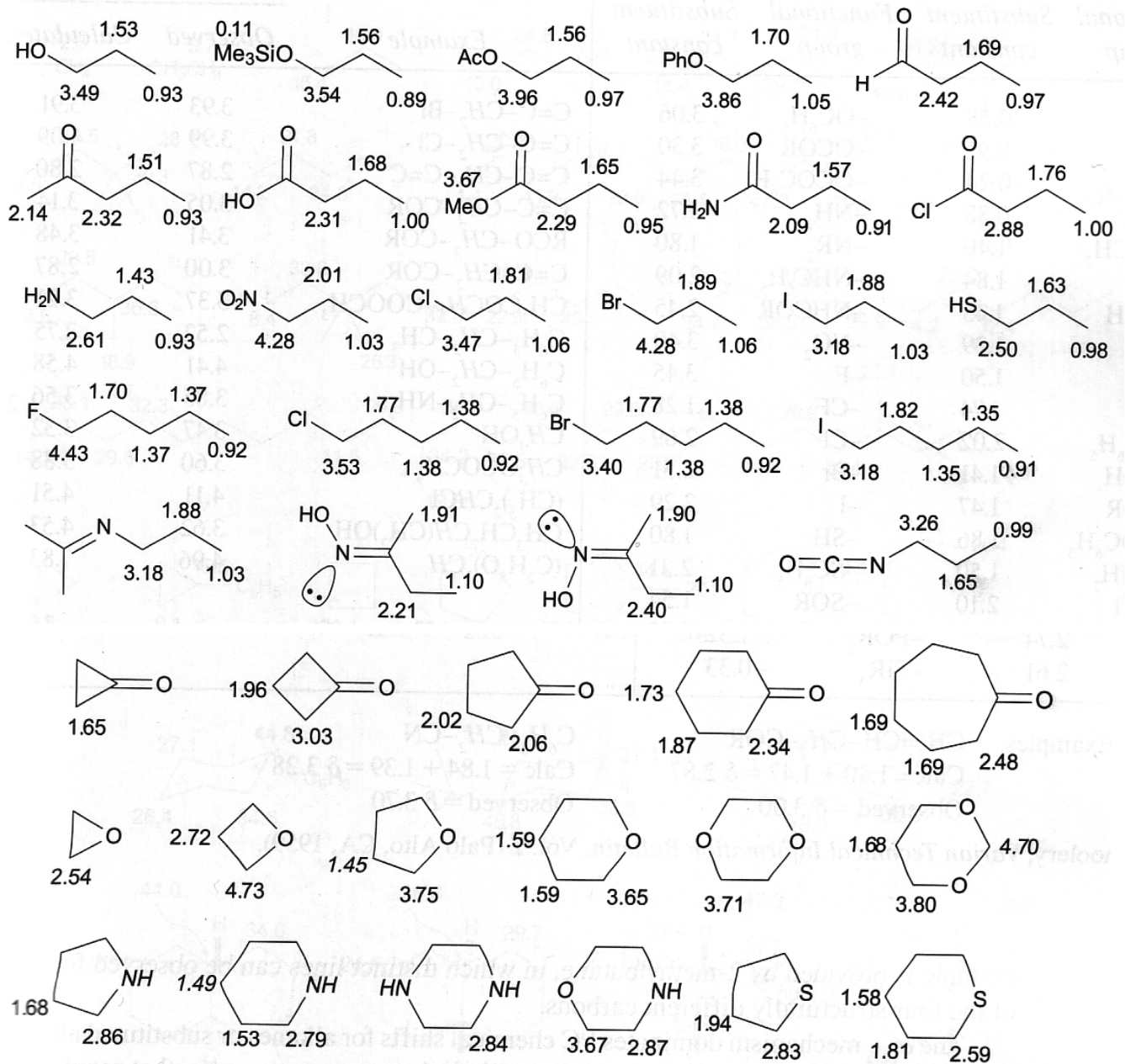
Substituted Alkanes



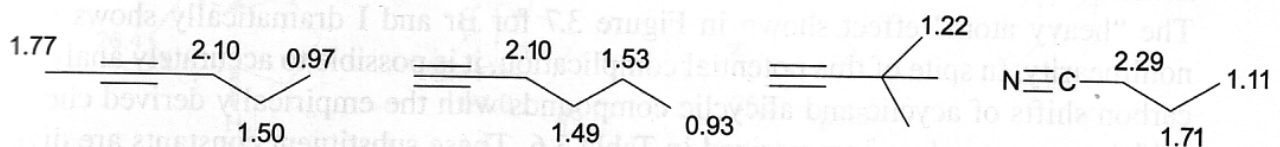
^1H NMR Tables

Experimental sp^3 ^1H chemical shifts (ppm) (cont.).

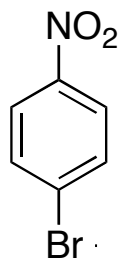
Functionalized Alkanes



Substituted Alkynes and C≡N



1. Calculate the chemical shifts for each of carbons in the following molecule. Place your answers on the line after the appropriate carbon atom. (9 points total)
Your answers must match the correct answer within +/- 1 ppm



Carbon a _____ ppm

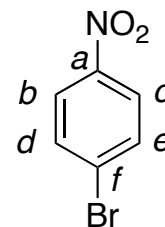
Carbon b _____ ppm

Carbon c _____ ppm

Carbon d _____ ppm

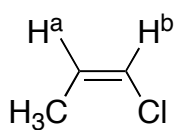
Carbon e _____ ppm

Carbon f _____ ppm



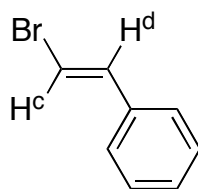
You may use the area below for scratch work, but it will not be graded

2. Calculate the chemical shifts for each of protons in the following molecules. Place your answers on the line after the appropriate carbon atom. (9 points total)
Your answers must match the correct answer within +/- 1 ppm



H^a _____ ppm

H^b _____ ppm

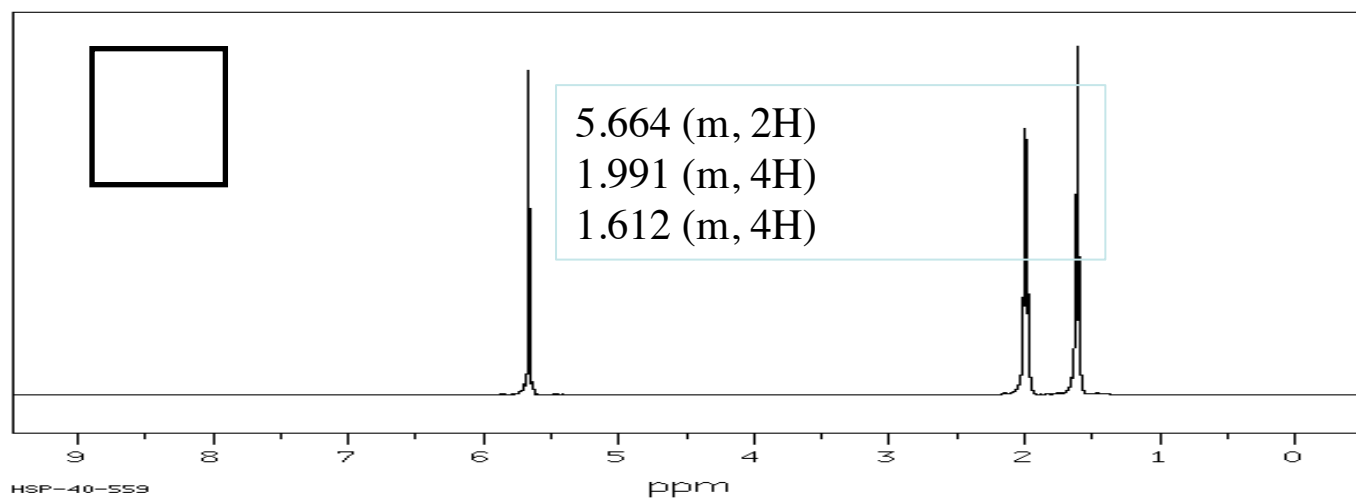
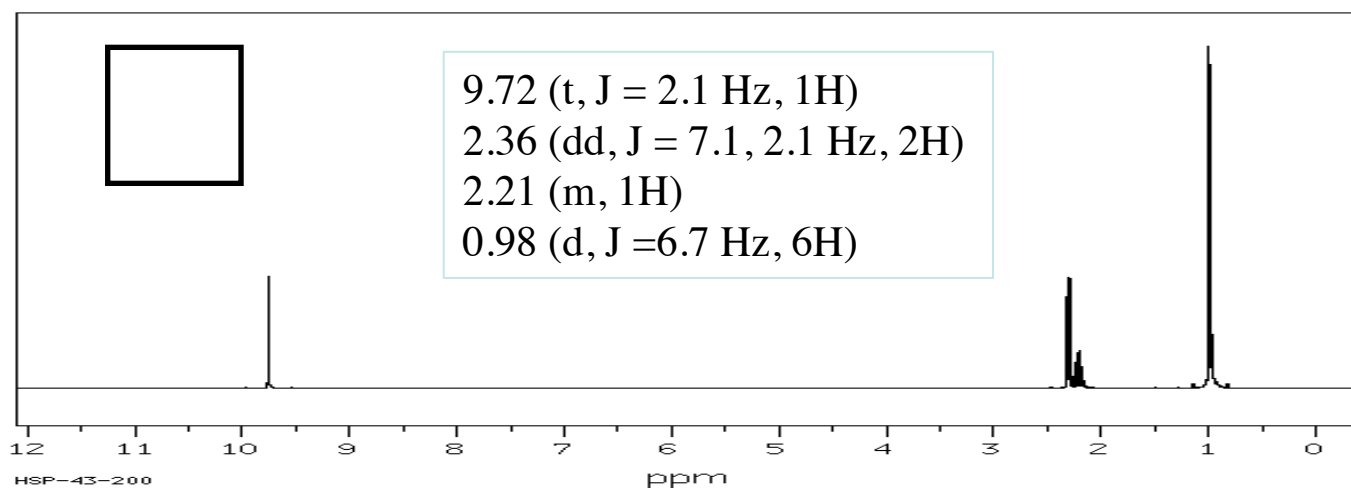
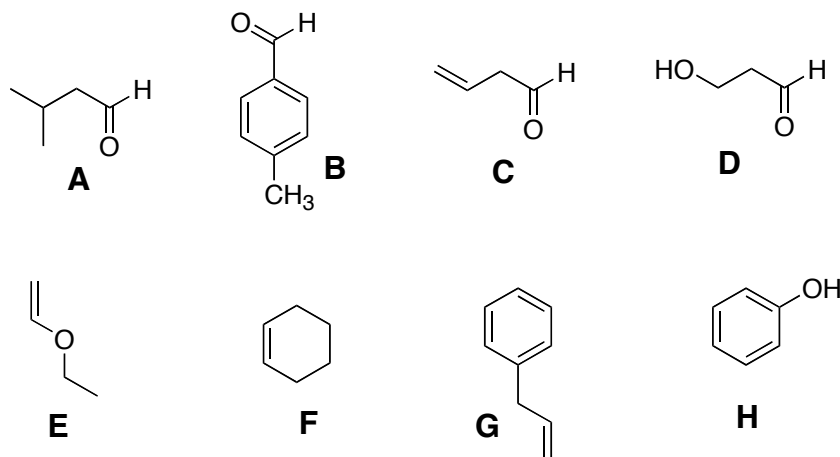


H^c _____ ppm

H^d _____ ppm

You may use the area below for scratch work, but it will not be graded

3. Match the following ^1H NMR spectra with one of the following substances. Write your answer in the box along side the spectrum. (6 points each)



4. Elucidate the following structure based on the ^{13}C NMR data



C^{13} NMR

173.4, s

51.5, q

33.1, t

32.9, t

32.0, t

23.5, t

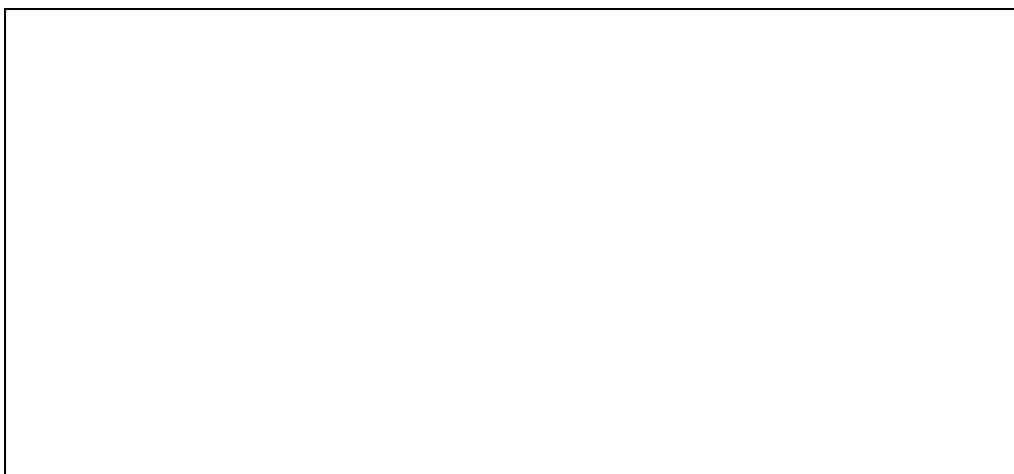
a) Calculate the IHD: _____ (1 point)

b) Show the substructure that is associated with the following ^{13}C NMR resonances (7 points)

173.4, s

51.5, q

c) Draw the structure (14 points)



5. Elucidate the following structure based on the following ^1H NMR and ^{13}C NMR data: $\text{C}_{10}\text{H}_{18}\text{O}_2$

^{13}C NMR

166.4, s
149.0, d
118.2, d
59.7, t
39.2, t
32.4, d
20.7, t
20.2, q
14.2, q
14.1, q

^1H NMR

5.92, dd, $J=7.9, 11.5$ Hz, 1H
5.68, d, $J=11.5$ Hz, 1H
4.15, q, $J=7.2$ Hz, 2H
2.40, m, 1H
1.27, t, $J=7.2$ Hz, 3H
1.2-1.3, m, 4H
0.99, d, $J=6.6$ Hz, 3H
0.88, t, $J=7.1$ Hz, 3H

a) Calculate the IHD: _____ (1 point)

b) Show the substructure that is associated with the following ^{13}C NMR resonances (5 points)

149.0, d
118.2, d

c) Show the substructure that is associated with the following ^{13}C NMR resonances (5 points)

166.4, s

d) Show the substructure that is associated with the following ^1H NMR resonances (5 points)

4.15, q, $J=7.2$ Hz, 2H

1.27, t, $J=7.2$ Hz, 3H

e) Show the substructure that is associated with the following ^1H NMR resonances. Be sure to comment on the significance of the 11.5 Hz coupling constant. (12 points)

5.92, dd, $J=7.9$, **11.5 Hz**, 1H

5.68, d, **$J=11.5$ Hz**, 1H

f) Show your final structure (20 points)

