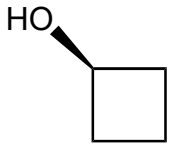
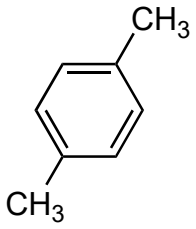
Organic Chemistry I, CHM 3140
Dr. Laurie S. Starkey, Cal Poly Pomona
Chapter 15 NMR, Part 1 - Practice Problems

For clicker question voting, go to:
https://pollev.com/lauriestarke263 or
text LAURIESTARKE263 to 37607

How many signals are expected for each compound?
Label each unique proton type (a/b/c).

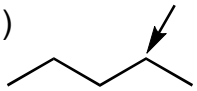




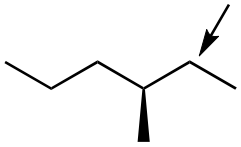
Describe the relationship of the indicated protons:

a) enantiotopic (one signal in NMR)
b) enantiotopic (separate signals in NMR)
c) diastereotopic (one signal in NMR)
d) diastereotopic (separate signals in NMR)
e) homotopic (one signal in NMR)

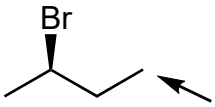
1)



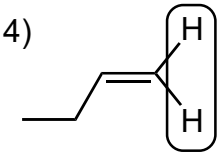
3)



2)



4)

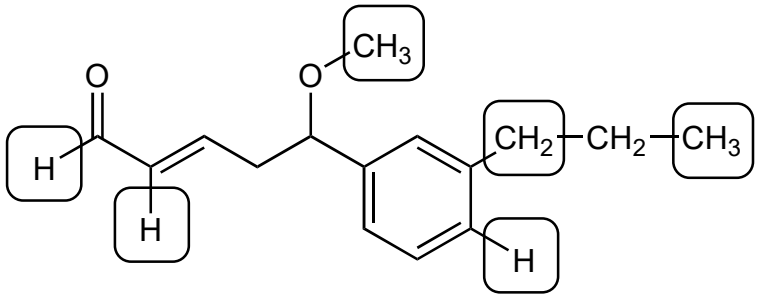


Match each highlighted proton with its approximate chemical shift:

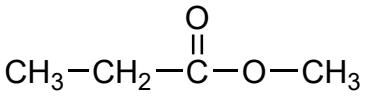
1, 2, 4, 5, 7, 10 ppm

Also, predict the splitting pattern for each highlighted proton.
Note: aldehyde protons typically do not couple with neighboring protons.

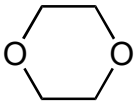
a) singlet (s)
b) doublet (d)
c) triplet (t)
d) quartet (q)
e) other



Predicting a ^{1}H NMR spectrum

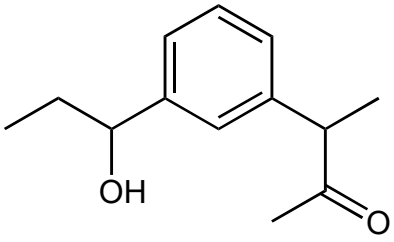


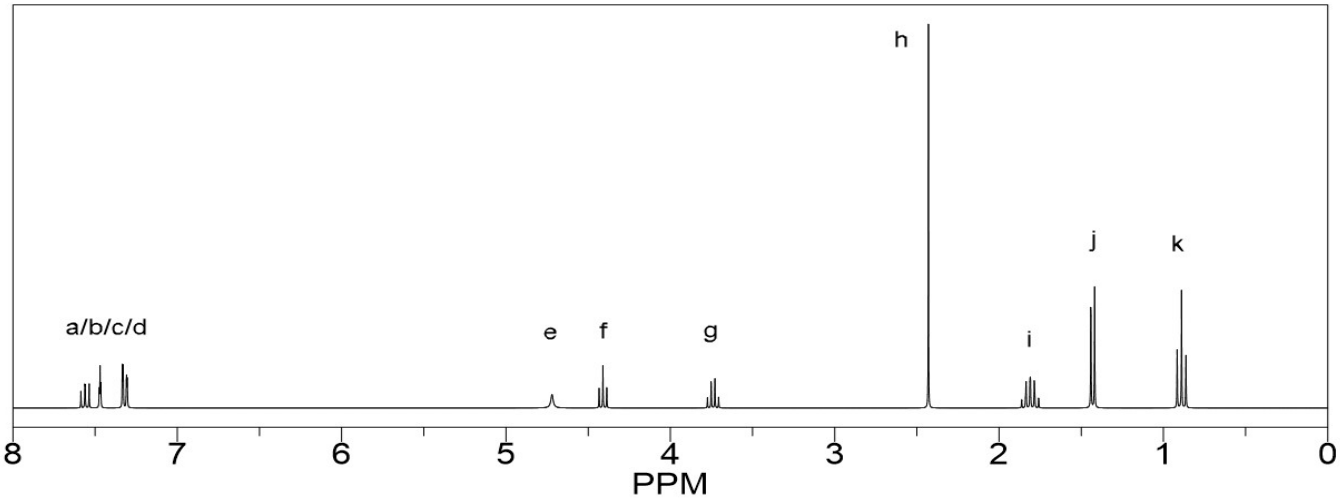
proton	#H, split	δ (ppm)*



proton	#H, split	δ (ppm)

Match the labeled peaks in the ^{1}H NMR with the protons on the given structure.



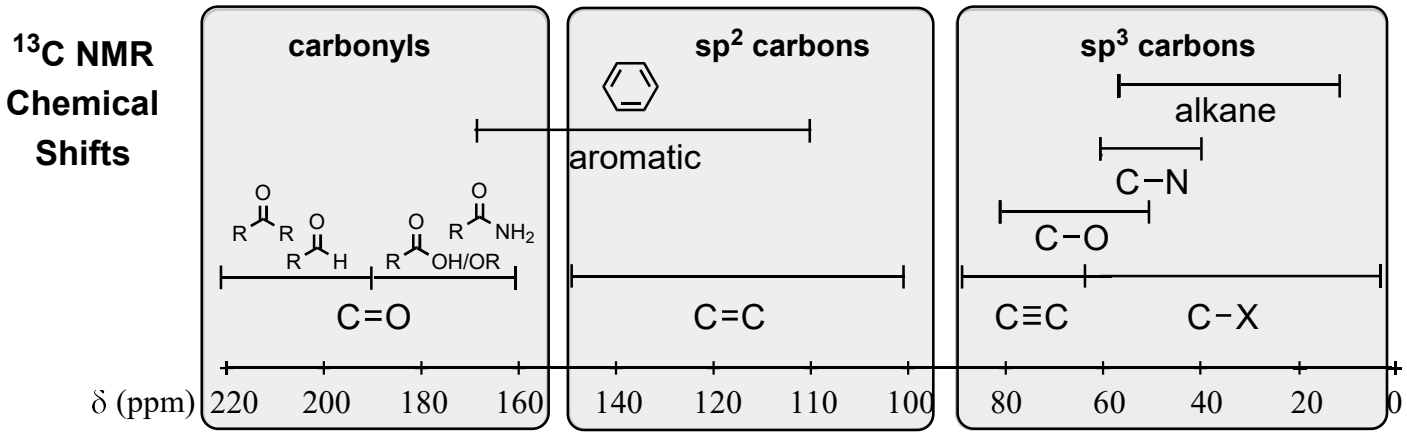


There are two isomeric carboxylic acids with the formula $C_3H_5O_2Cl$.
Provide a structure that matches each set of ^{1}H NMR data.

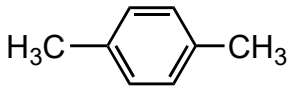
Isomer A	**Isomer B**
1.7 ppm 3H d	2.9 ppm 2H t
4.4 ppm 1H q	3.8 ppm 2H t
12.4 ppm 1H s	11.7 ppm 1H s

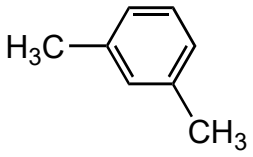
Interpreting ^{13}C NMR Spectra (Klein section 15.12)

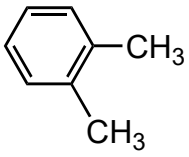
- one signal for each unique carbon type
- chemical shifts ~ 0 to 220 ppm
- signals are typically all singlets ("proton-decoupled" or "broadband decoupled")
- # of hydrogens attached to each carbon can be determined by DEPT experiment
  (*see Klein 15.13 and SkillBuilder 15.10, but we will not be covering DEPT in CHM 3140*)
- ^{13}C isotope ~1% of carbon atoms, so ^{13}C NMR requires more sample and/or more scans



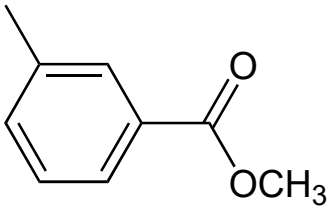
How could you use ^{13}C NMR to distinguish between the three isomers of dimethylbenzene?



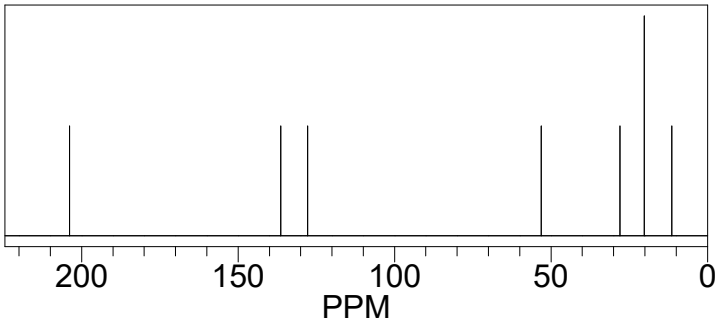




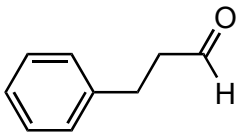
Predict the number of ^{13}C NMR signals (label a/b/c) and the approximate chemical shifts for each.



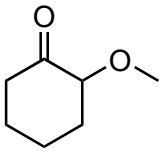
Each of the compounds shown has seven signals in its ^{13}C NMR spectrum.
Which structure matches the spectrum provided? Explain



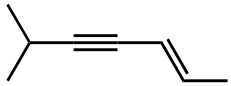
A



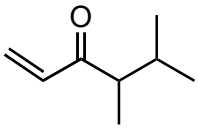
B



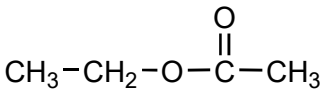
C

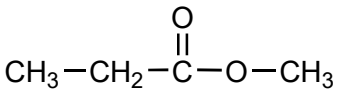


D



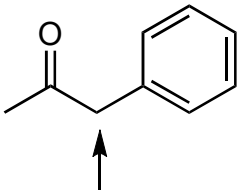
Which would be better to distinguish the following compounds, ^{1}H or ^{13}C NMR (or are they equally suitable)? Explain, and describe the peak(s) to look for.





What is the expected splitting pattern for the indicated protons?

Do you predict the chemical shift to be closer to
δ = 2.5 ppm or δ = 3.5 ppm? Explain



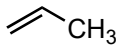
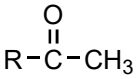
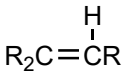
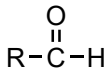
Draw the dichloropentane isomer that has exactly two ^{1}H NMR signals.

Chapter 15 textbook problems for Exam II:
SkillBuilders 15.1-15.7 (^{1}H NMR) and 15.9 (^{13}C)
Do the following problems: 1-22, 26, 35-39, 41, 42, 45, 47, 48, 50, 63-71.
Exam III (interpreting ^{1}H NMR spectra): SkillBuilder 15.8 and problems: 23-25, 57-59, 64.

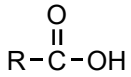
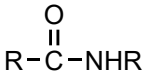
Cal Poly Pomona, Dr. L. S. Starkey

^{1}H and ^{13}C NMR - General Chemical Shifts

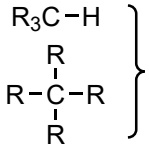
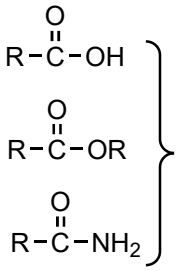
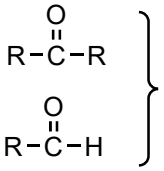
^{1}H NMR: Protons on Carbon

Type of C-H	δ (ppm)	Description
$R-CH_3$	0.9	alkyl (methyl)
$R-CH_2-R$	1.3	alkyl (methylene)
R_3C-H	1.5-2	alkyl (methine)
	1.8	allylic
	2-2.3	α to carbonyl
$Ar-CH_3$	2.3	benzylic
$RC\equiv C-H$	2.5	alkynyl
R_2N-CH_3	2-3	α to nitrogen
$R-CH_2-X$	3-3.5	α to halogen
$RO-CH_3$	3.8	α to oxygen
$R-CH_2-F$	4.5	α to fluorine
	5-5.3	vinylic
$Ar-H$	7.3	aromatic
	9.7	aldehyde

^{1}H NMR: Protons on Oxygen/Nitrogen

Type of H	δ (ppm)	Description
ROH	0.5-5	alcohol
ArOH	4-7	phenol
	10-13	carb. acid
RNH_2	0.5-5	amine
$ArNH_2$	3-5	aniline
	5-9	amide

^{13}C NMR: Carbon atoms

Type of carbon	δ (ppm)	Description
$R-CH_3$	10-30	methyl
$R-CH_2-R$	15-55	methylene
	20-60	methine or quaternary
$C-I$	0-40	
$C-Br$	25-65	
$C-N$	40-60	
$C-Cl$	35-80	
$C-O$	40-80	
$RC\equiv CR$	65-90	alkynyl
$R_2C=CR_2$	100-150	alkenyl
	110-170	aromatic
	165-185	C=O, carboxylic acid, ester, amide
	185-220	C=O, ketone or aldehyde

R = alkyl group

Ar = aromatic ring, such as a benzene ring