

Chem 333, Exam 1
Professor Fox
FALL 2013

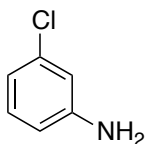
Your Name _____

- Q1) 12 points
- Q2) 12 points
- Q3) 16 points
- Q4) 25 points
- Q5) 33 points

tables at back of exam

B

1. Calculate the chemical shifts for each of the carbons in the following molecule. Place your answers on the line after the appropriate carbon atom. A correct answer should be precise to one decimal place (e.g. 128.5; NOT 129 ppm)
 Your answers must match the correct answer within +/- 0.5 ppm
 (12 points total)



Carbon a _____ ppm

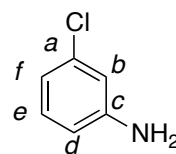
Carbon b _____ ppm

Carbon c _____ ppm

Carbon d _____ ppm

Carbon e _____ ppm

Carbon f _____ ppm

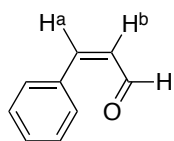


You may use the area below for scratch work, but it will not be graded

2. Calculate the chemical shifts for each of the labeled protons in the following molecules. Place your answers on the line after the appropriate atom. A correct answer should be precise to two decimal places (e.g. 5.25 ppm; NOT 5.3 ppm)

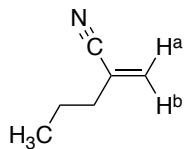
Your answers must match the correct answer within ± 0.05 ppm

(12 points total)



H^a _____

H^b _____

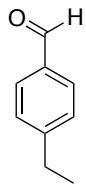


H^a _____

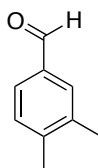
H^b _____

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

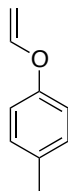
3. Match the following ^1H NMR spectra with one of the following substances. Write your answer in the box along side the spectrum. (8 points each)



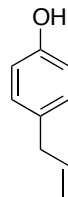
A



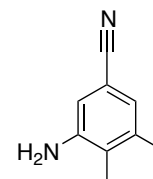
B



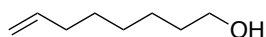
C



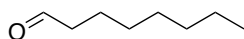
D



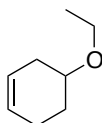
E



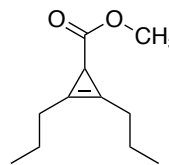
F



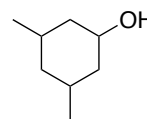
G



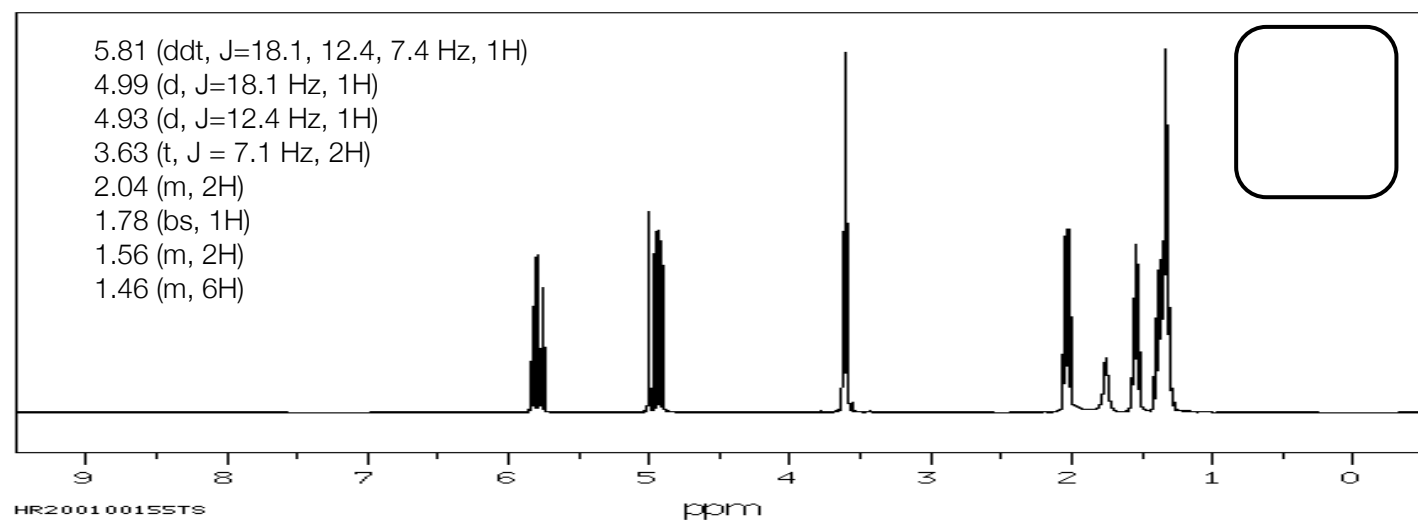
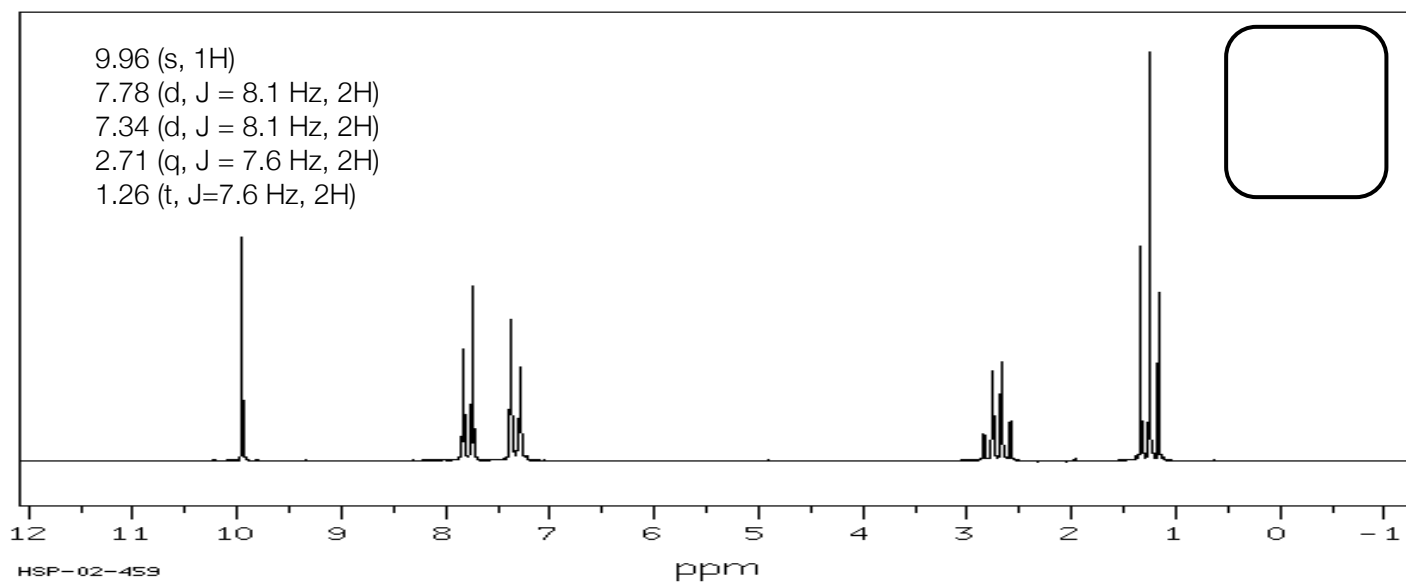
H



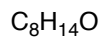
I



J



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







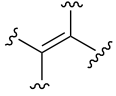




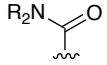


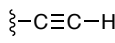
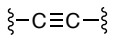


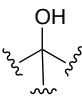



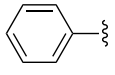
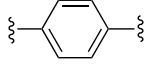
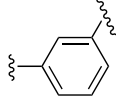
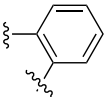
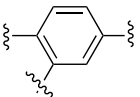
145.3, d
 112.6, t
 72.5, s
 39.9, t (2 carbons)
 22.0, t
 21.5, t (2 carbons)

a) Calculate the IHD: _____ (1 pt)

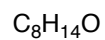
b) How many hydrogens are on carbons? _____ (1 pt)

c) Circle the substructure that is associated with the following ^{13}C NMR resonances. If none of the below functional groups exist, then circle "none of the above" (6 points)

145.3 d
 112.6, t

								
mono-substituted alkene	cis-disubstituted alkene	trans-disubstituted alkene	trisubstituted alkene	tetrasubstituted alkene				
								
	ketone	aldehyde	acid	ester	amide	nitro	nitrile	
								
terminal alkyne	internal alkyne	primary alcohol	secondary alcohol	tertiary alcohol	primary amine	secondary amine	tertiary amine	
								
monosubstituted benzene	1,4-disubstituted benzene	1,3-disubstituted benzene	1,2-disubstituted benzene	trisubstituted benzene				
none of the above								

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



145.3, d

112.6, t

72.5, s

39.9, t (2 carbons)

22.0, t

21.5, t (2 carbons)

d) Identify the functional group associated with 72.5, s.

If the correct functional group is not listed, then circle "none of the above" (6 points)



mono-substituted alkene



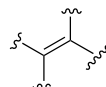
cis-disubstituted alkene



trans-disubstituted alkene



trisubstituted alkene



tetrasubstituted alkene



ketone



aldehyde



acid



ester



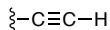
amide



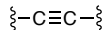
nitro



nitrile



terminal alkyne



internal alkyne



primary alcohol



secondary alcohol



tertiary alcohol



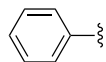
primary amine



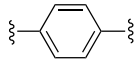
secondary amine



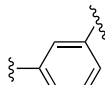
tertiary amine



monosubstituted benzene



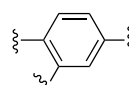
1,4-disubstituted benzene



1,3-disubstituted benzene



1,2-disubstituted benzene



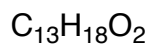
trisubstituted benzene

none of the above

e) Draw the structure (11 points)



5. Elucidate the following structure based on the ^1H and ^{13}C NMR data (continued)



^1H NMR

7.70 ppm (d, $J=8.0$ Hz, 2H)
 6.91 ppm (d, $J=8.0$ Hz, 2H)
 3.86 ppm (m, 1H)
 2.45 (s, 3H)
 1.67 (m, 2H)
 1.43 (d, $J=7.2$ Hz, 3H)
 1.33 (m, 2H)
 0.96 (t, $J=6.9$ Hz, 3H)

^{13}C NMR





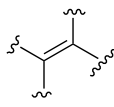




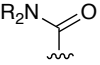


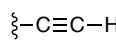
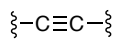


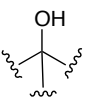



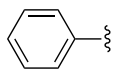
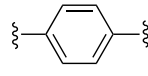
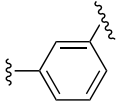
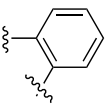
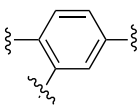
197 (s)
 163 (s)
 129 (s)
 128 (2 carbons, d)
 114 (2 carbons, d)
 73 (d)
 39 (t)
 23 (q)
 20 (q)
 17(t)
 14 (q)

a) Calculate the IHD: _____ (1 pt)

b) How many hydrogens are on carbons? _____ (1 pt)

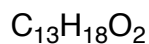
c) Identify the substructure that is associated with the following. (6 pts)

197 (s)

										
mono-substituted alkene	cis-disubstituted alkene	trans-disubstituted alkene	trisubstituted alkene	tetrasubstituted alkene						
										
ketone	aldehyde	acid	ester	amide	nitro	nitrile				
										
terminal alkyne	internal alkyne	primary alcohol	secondary alcohol	tertiary alcohol	primary amine	secondary amine	tertiary amine			
										
monosubstituted benzene	1,4-disubstituted benzene	1,3-disubstituted benzene	1,2-disubstituted benzene	trisubstituted benzene						

none of the above

5. Elucidate the following structure based on the ^1H and ^{13}C NMR data



^1H NMR

7.70 ppm (d, $J=8.0$ Hz, 2H)
 6.91 ppm (d, $J=8.0$ Hz, 2H)
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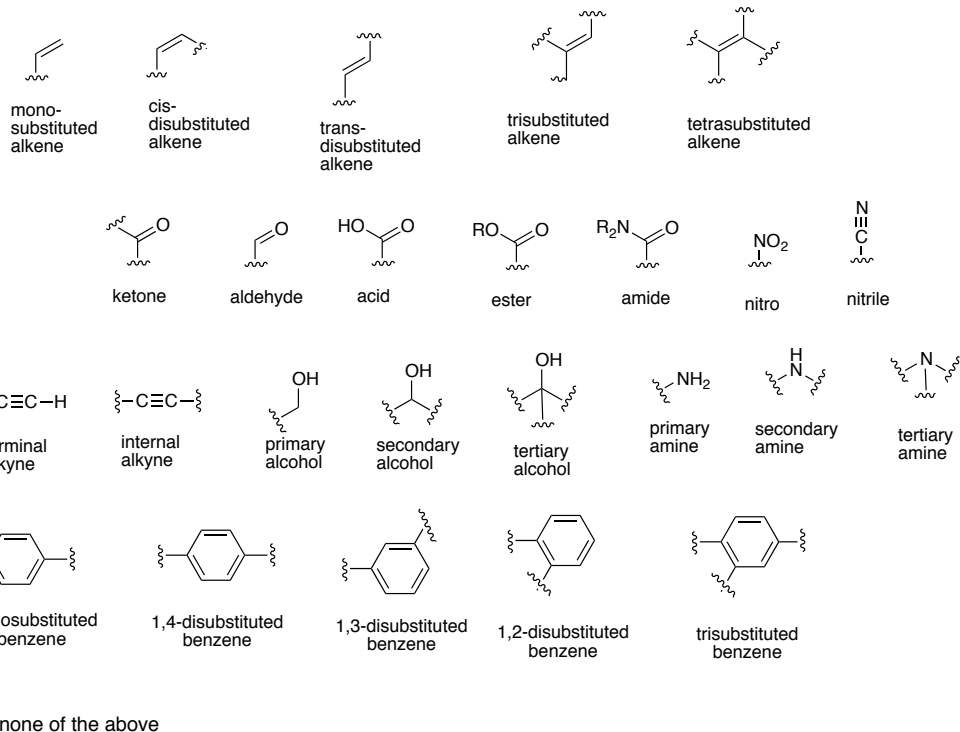
^{13}C NMR

197 (s)
 163 (s)
 129 (s)
 128 (2 carbons, d)
 114 (2 carbons, d)
 73 (d)
 39 (t)
 23 (q)
 20 (q)
 17(t)
 14 (q)

d) Identify the substructure that is associated with the following. (7 points)

7.70 ppm (d, $J=8.0$ Hz, 2H)

6.91 ppm (d, $J=8.0$ Hz, 2H)



e) Draw the structure (18 points)

