

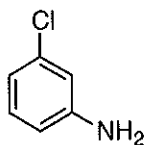
Chem 333, Exam 1
Professor Fox
FALL 2013

Your Name Key.

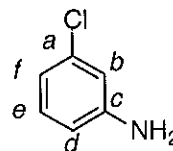
- Q1) 12 points
- Q2) 12 points
- Q3) 16 points
- Q4) 25 points
- Q5) 33 points

tables at back of exam

1. Calculate the chemical shifts for each of 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 136.2 ppm
 Carbon b 116.3 ppm
 Carbon c 148.7 ppm
 Carbon d 114.1 ppm
 Carbon e 130.8 ppm
 Carbon f 119.2 ppm



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

$$C^a = 128.5 (+6.4) (+1.3) = 136.2$$

C1-Cl C3-NH₂

$$C^b = 128.5 (+0.2) (-12.4) = 116.3$$

C2-Cl C2-NH₂

$$C^c = 128.5 (+1.0) (+19.2) = 148.7$$

C3-Cl C1-NH₂

$$C^d = 128.5 (-2.0) (-12.4) = 114.1$$

C4-Cl C2-NH₂

$$C^e = 128.5 (+1.0) (+1.3) = 130.8$$

C3-Cl C3-NH₂

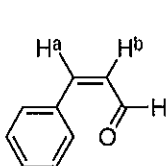
$$C^f = 128.5 (+0.2) (-9.5) = 119.2$$

C2-Cl C4-NH₂

2. Calculate the chemical shifts for each of 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)

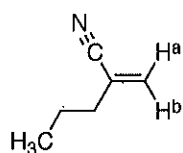
Your answers must match the correct answer within ± 0.05 ppm

(12 points total)



H^a 7.81

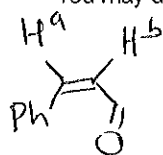
H^b 6.18



H^a 5.74

H^b 5.57

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

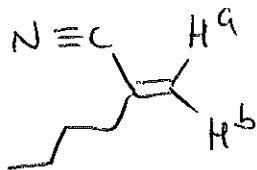


$$H^a = 5.25 (+1.35) (+1.21) = 7.81$$

gem trans
aromatic aldehyde

$$H^b = 5.25 (+1.03) (-0.10) = 6.18$$

gem trans
aldehyde Aromatic



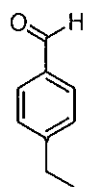
$$H^a = 5.25 (+0.78) (-0.29) = 5.74$$

cis trans
-C≡N alkyl

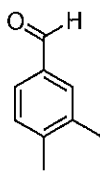
$$H^b = 5.25 (+0.58) (-0.26) = 5.57$$

trans cis
-C≡N alkyl

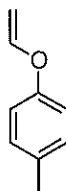
3. Match the following ^1H NMR spectra with one of the following substances. Write your answer in the box along side the spectrum. (8 points each)



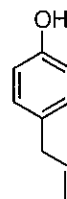
A



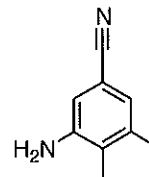
B



C



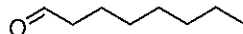
D



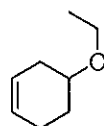
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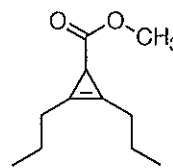
F



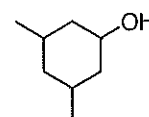
G



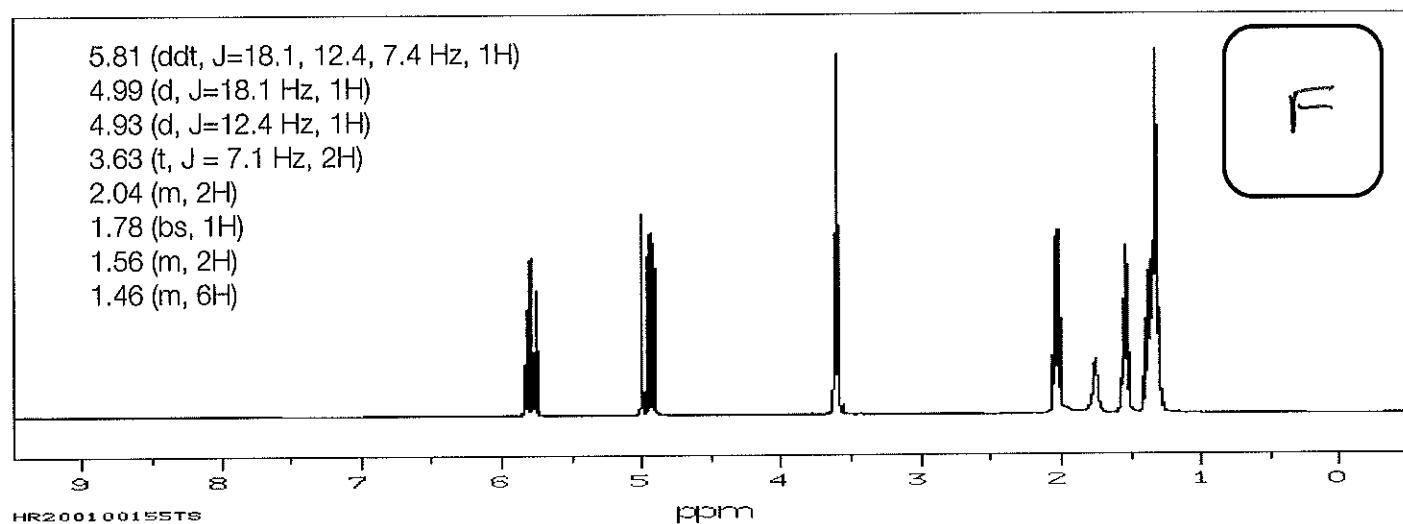
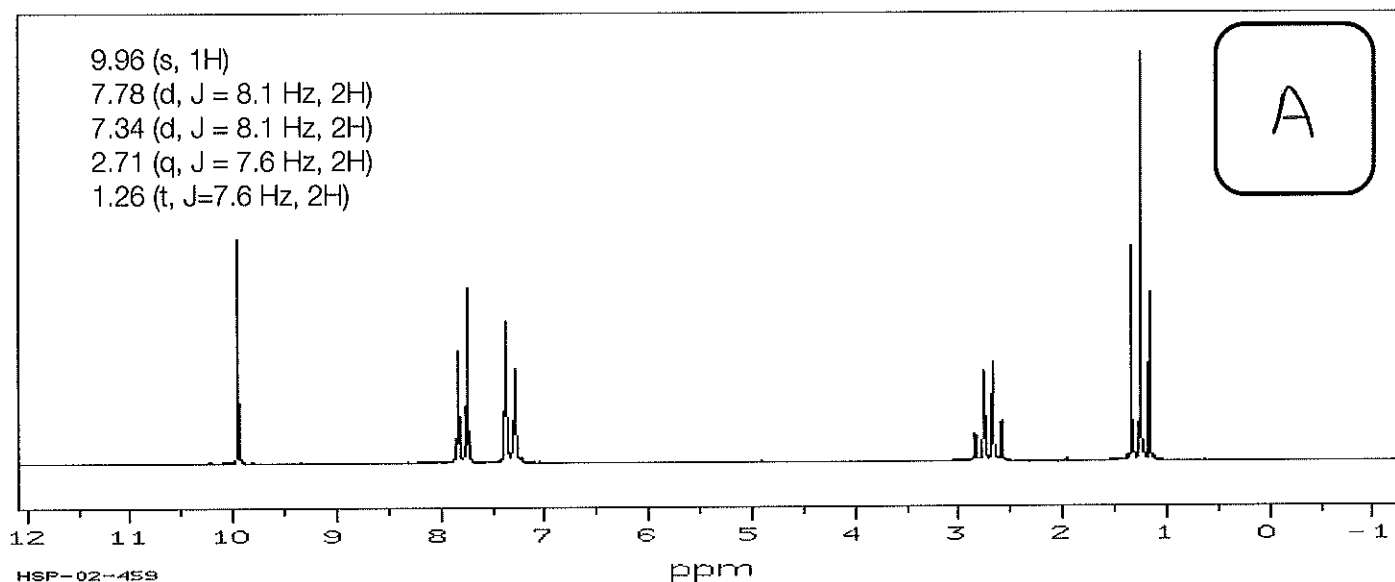
H



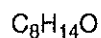
I



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)

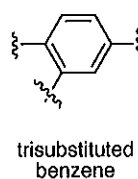
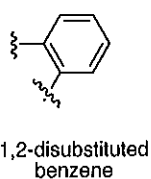
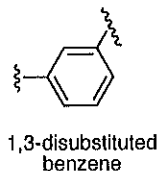
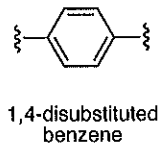
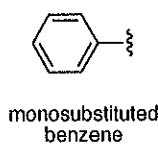
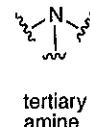
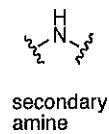
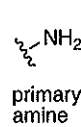
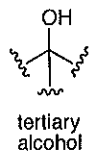
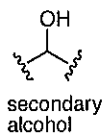
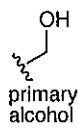
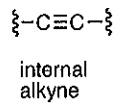
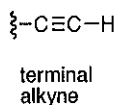
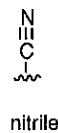
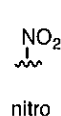
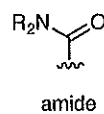
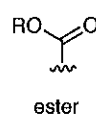
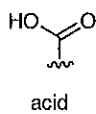
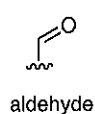
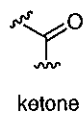
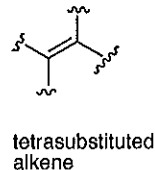
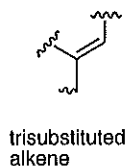
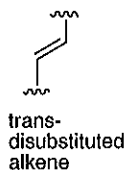
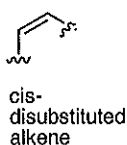
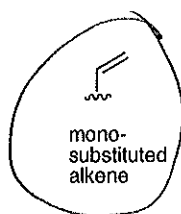
a) Calculate the IHD: 2 (1 pt)

b) How many hydrogens are on carbons? 13 (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)

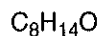
145.3 d

112.6, t



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

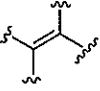
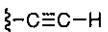
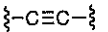
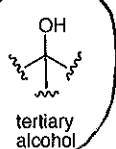
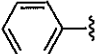
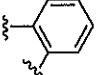
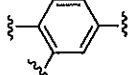
39.9, t (2 carbons)

22.0, t

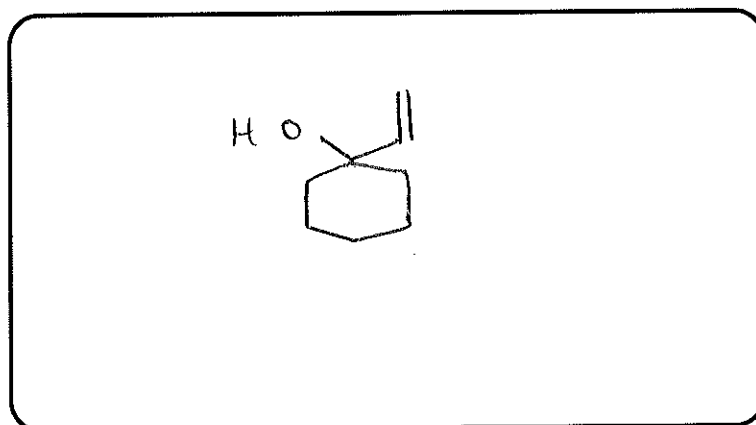
21.5, t (2 carbons)

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

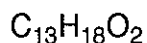
If the correct functional group is not listed, then circle "none of the above" (6 points)

						
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
						
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

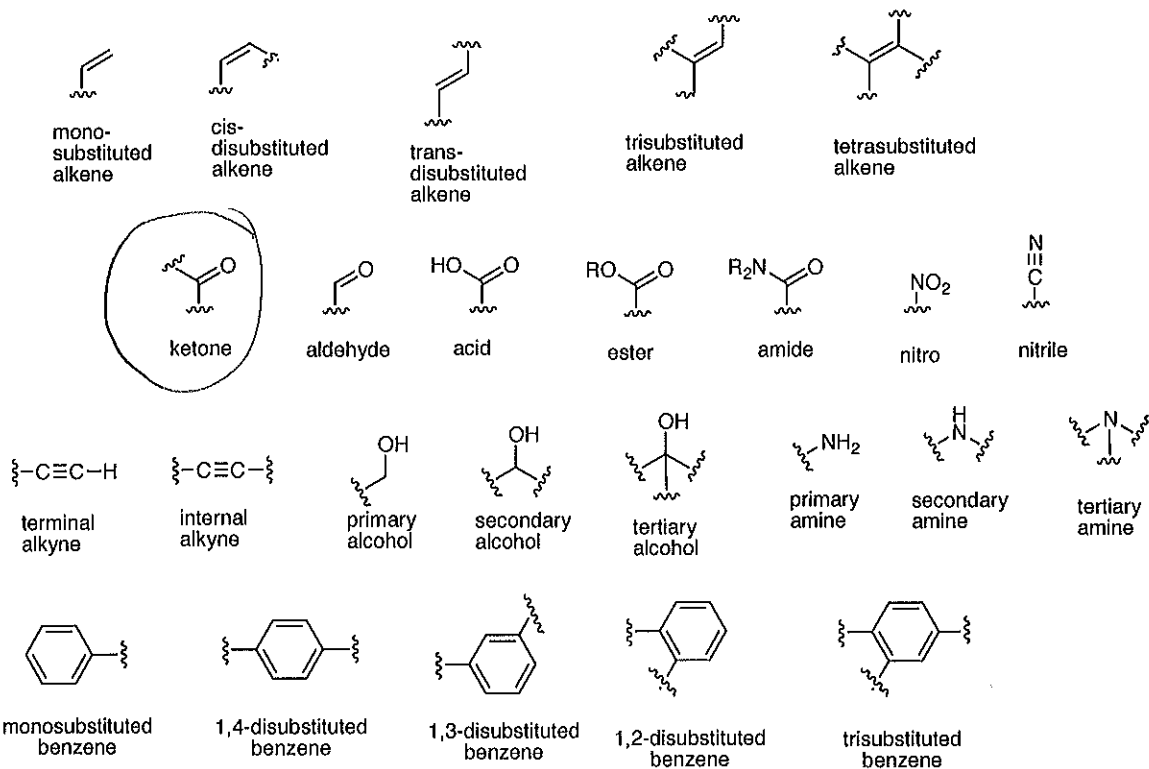
197 (s)
 163 (s)
 129 (s)
 128 (2 carbons, d)
 114 (2 carbons, d)
 73 (d)
 39 (t)
 23 (q)
 20 (q)
 17(t)
 14 (q)

a) Calculate the IHD: 5 (1 pt)

b) How many hydrogens are on carbons? 18 (1 pt)

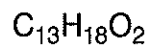
c) Identify the substructure that is associated with the following. (6 pts)

197 (s)



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)
 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)

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)



mono-substituted alkene



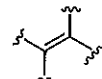
cis-disubstituted alkene



trans-disubstituted alkene



trisubstituted alkene



tetrasubstituted alkene



ketone



aldehyde



acid



ester



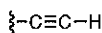
amide



nitro



nitrile



terminal alkyne



internal alkyne



primary alcohol



secondary alcohol



tertiary alcohol



primary amine



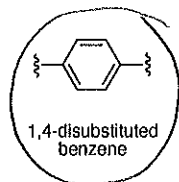
secondary amine



tertiary amine



monosubstituted benzene



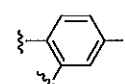
1,4-disubstituted benzene



1,3-disubstituted benzene



1,2-disubstituted benzene



trisubstituted benzene

none of the above

e) Draw the structure (18 points)

