

Chem 334, Exam 2
Professor Fox
Spring 2009

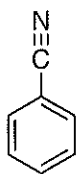
Your Name key

Your TA's Name _____

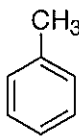
- Question 1, 3 points each
- Question 2, 12 points
- Question 3, 12 points
- Question 4a, 10 points
- Question 4b, 10 points
- Question 4c, 10 points
- Question 4d, 10 points
- Question 4e, 18 points

key

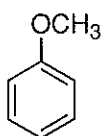
1. Match the following compounds with their ^{13}C NMR spectra. Note: only chemical shift data is given [multiplicities (s,d,t,q) are not needed to solve this problem]



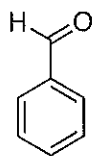
A



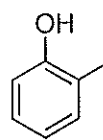
B



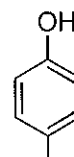
C



D

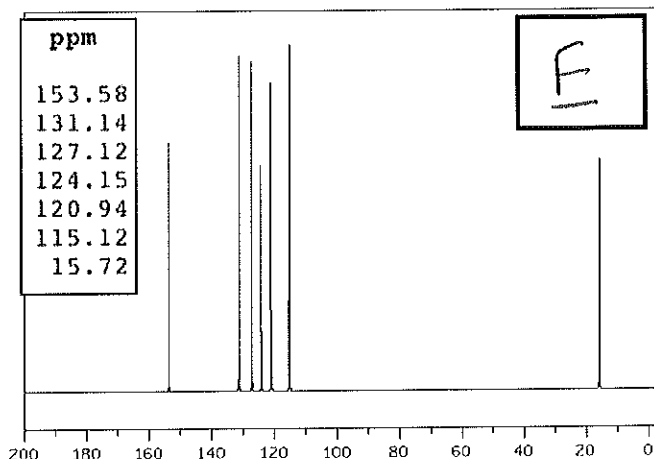
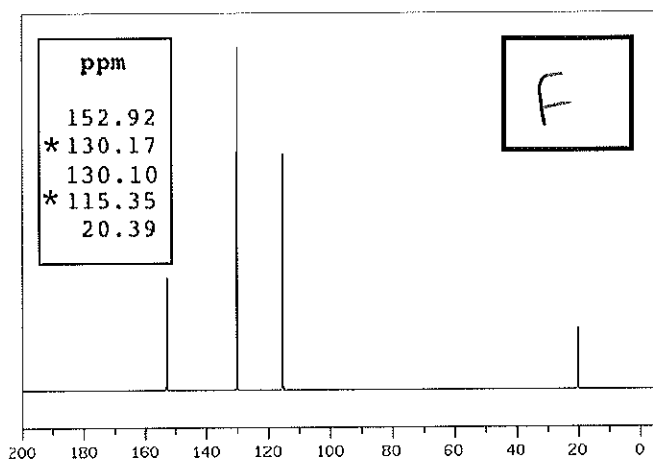
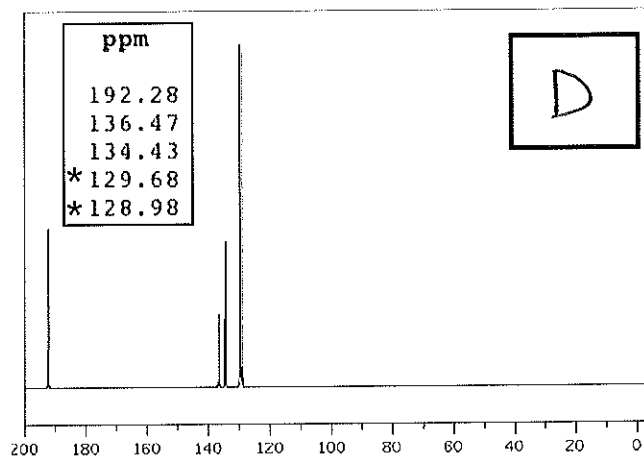
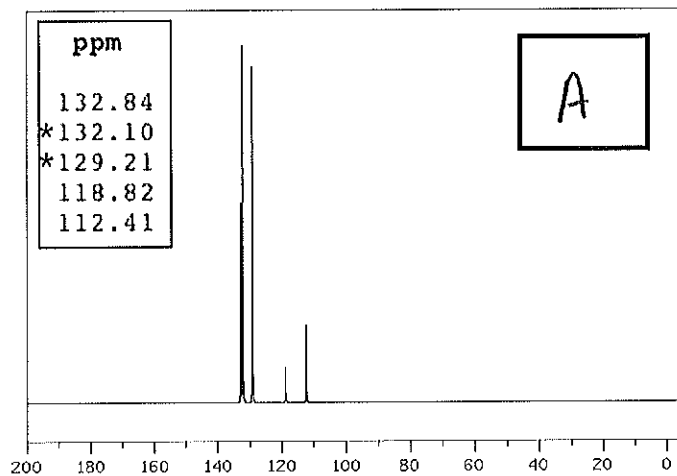
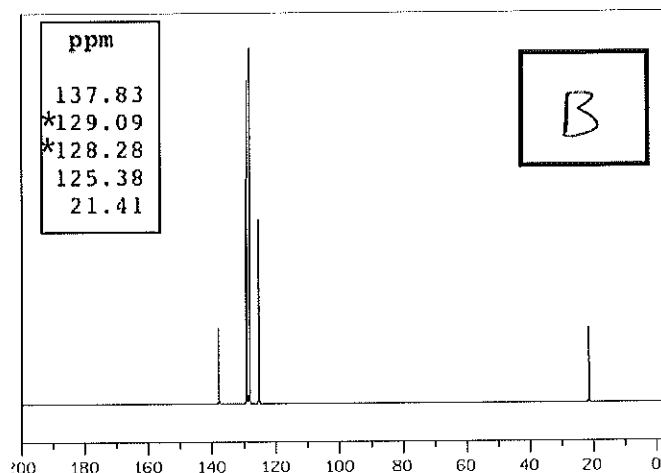
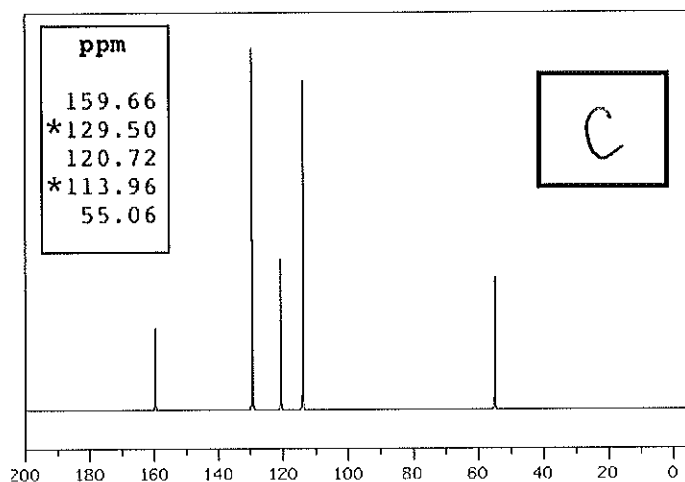


E



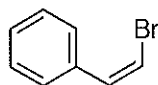
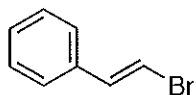
F

Note: * = 2 carbons

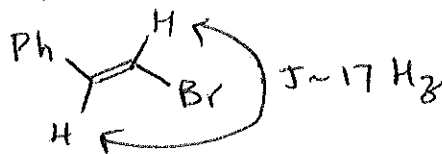


key.

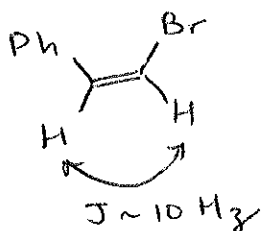
2. Explain how you would use ^1H NMR spectroscopy to distinguish the following compounds. You may use chemical structures to support your answer, but use no more than 30 words.



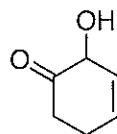
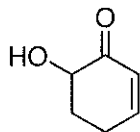
TRANS ALKENE : expect $J \sim 17 \text{ Hz}$



CIS ALKENE : expect $J \sim 10 \text{ Hz}$



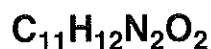
3. Explain how you would use IR spectroscopy to distinguish the following compounds. You may use chemical structures to support your answer, but use no more than 30 words.



α, β UNSATURATED
ketone : expect
 $\sim 1685 \text{ cm}^{-1}$

UNCONJUGATED ketone :
expect $\sim 1715 \text{ cm}^{-1}$

4. Elucidate the following structure

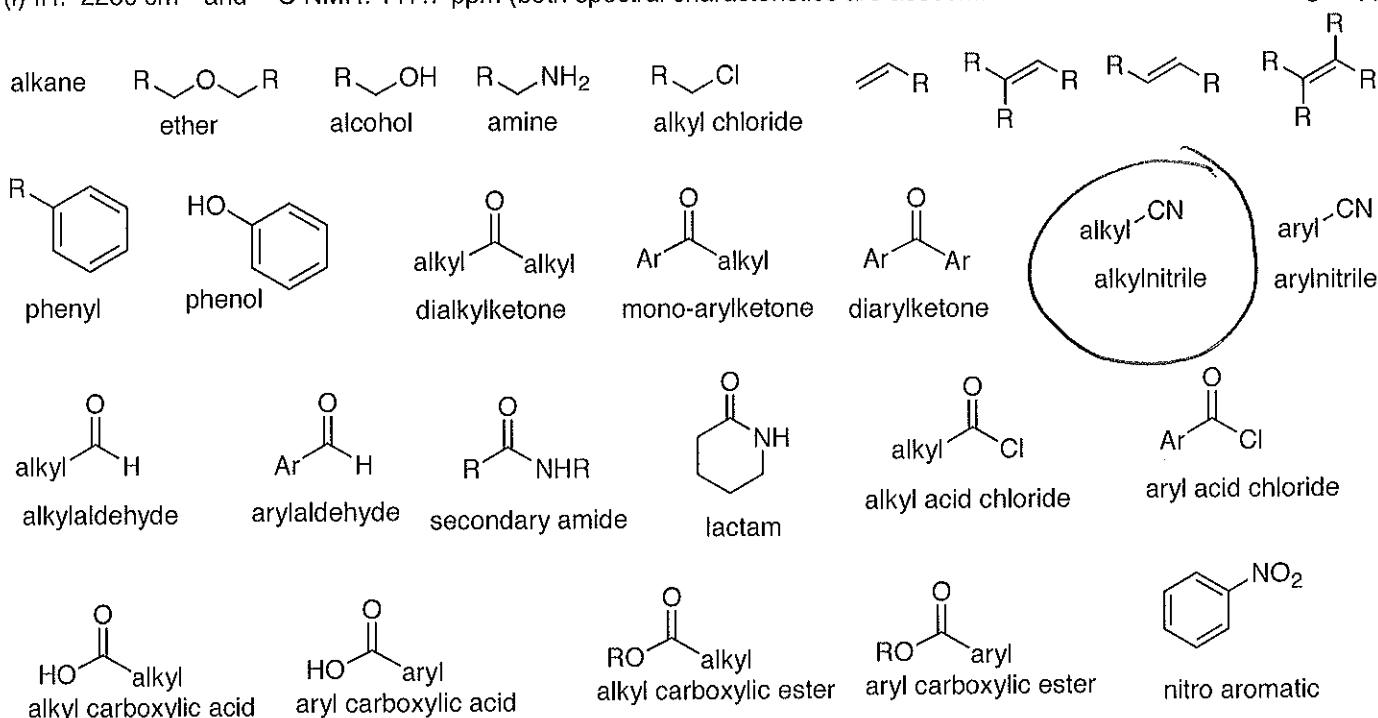


¹³ C NMR	¹ H NMR	IR (cm ⁻¹)
168.2 (s)	8.0 (br s, 1H)	3600-3300 (br)
139.7 (s)	7.57 (d, J=7.7 Hz, 2H)	2260
136.5 (s)	7.17 (d, J=7.7 Hz, 2H)	1690
127.5 (d, 2 carbons)	4.50 (dd, J=7.9, 6.5 Hz, 1H)	1530
120.5 (d, 2 carbons)	2.89 (dd, J=7.9, 4.0 Hz, 1H)	
117.7 (s)	2.78 (dd, J=6.5, 4.0 Hz, 1H)	
70.3 (d)	2.02 (s, 3H)	
28.0 (t)	1.98 (bs, 1H)	
17.6 (q)		(IR taken with dilute sample)

a) Circle the functional group that is associated with

note: "Ar" refers to aryl, or an aromatic ring

(i) IR: 2260 cm⁻¹ and ¹³C NMR: 117.7 ppm (both spectral characteristics are associated with the same functional group)



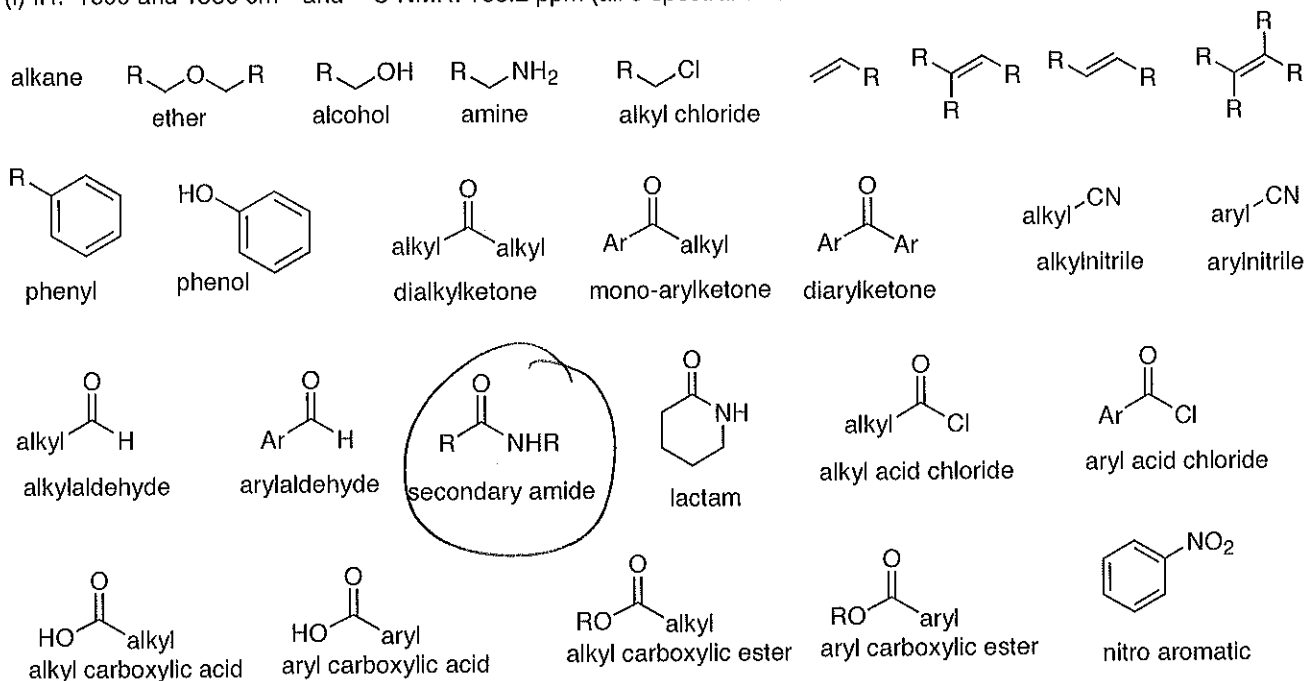
key.

4. Elucidate the following structure

b) Circle the functional group that is associated with

note: "Ar" refers to aryl, or an aromatic ring

(i) IR: 1690 and 1530 cm^{-1} and ^{13}C NMR: 168.2 ppm (all 3 spectral characteristics are associated with the same functional group)

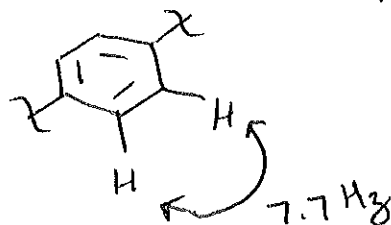


c) Identify the substructure that is associated with the following. Rationalize your answer based both on the chemical shifts and the coupling constants:

7.57 (d, $J=7.7\text{ Hz}$, 2H)

7.17 (d, $J=7.7\text{ Hz}$, 2H)

p-substituted
benzene



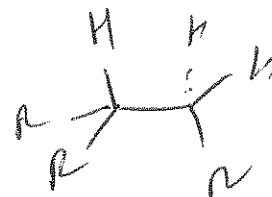
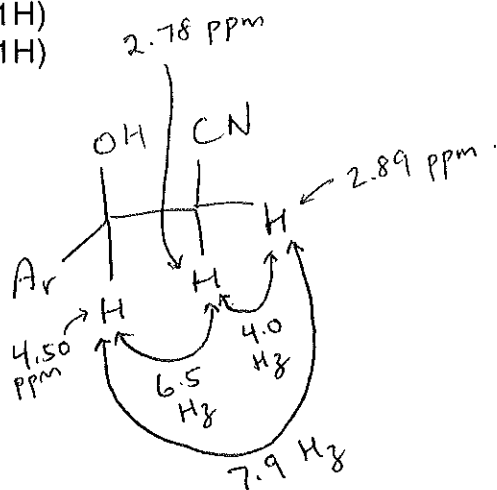
key.

d. Assign the following coupling constants. Your answer must clearly indicate which protons are coupled to one another.

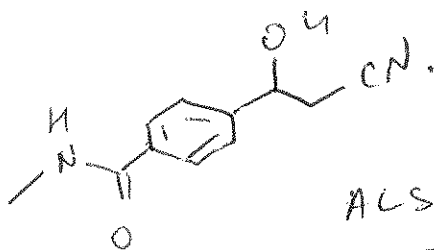
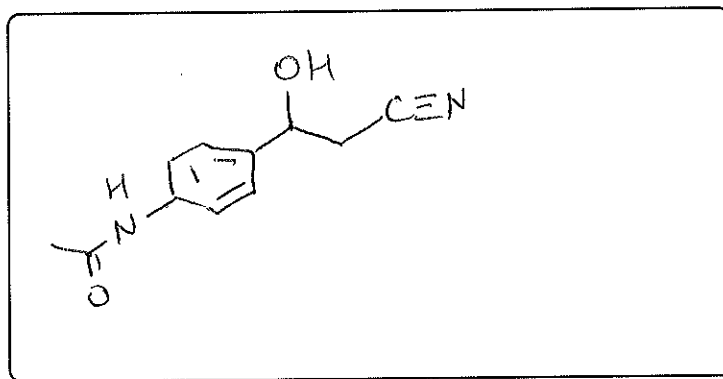
4.50 (dd, $J=7.9, 6.5$ Hz, 1H)

2.89 (dd, $J=7.9, 4.0$ Hz, 1H)

2.78 (dd, $J=6.5, 4.0$ Hz, 1H)



e) draw the structure of the product (no partial credit)



ALSO Accepted. (18 pts)