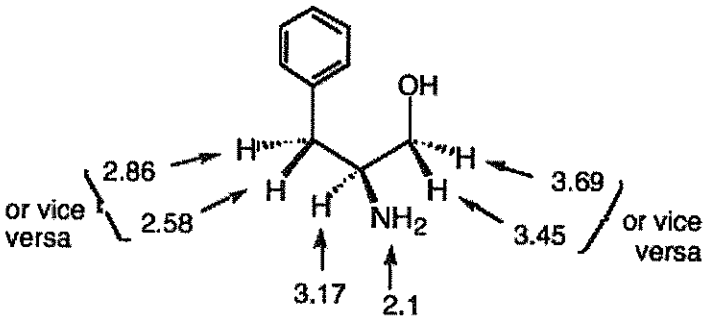
Chem 334, Exam 1
Professor Fox
Spring 2010

Your Name key

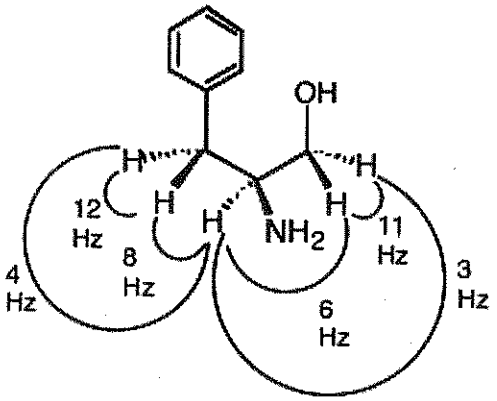
Open note, open book

For questions 4b and 5b, please use the following as an example for formatting your answers

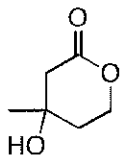
^{1}H assignments



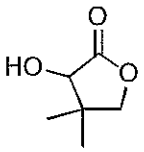
$J_{H\text{-}H}$ assignments



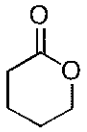
1. Match the following to their IR spectra. (15 points) (not all compounds have a match). Place an X next to compounds without a match



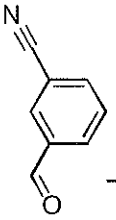
A



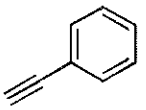
B

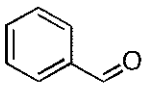


X

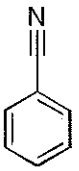


D

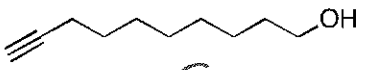

X



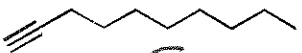
X



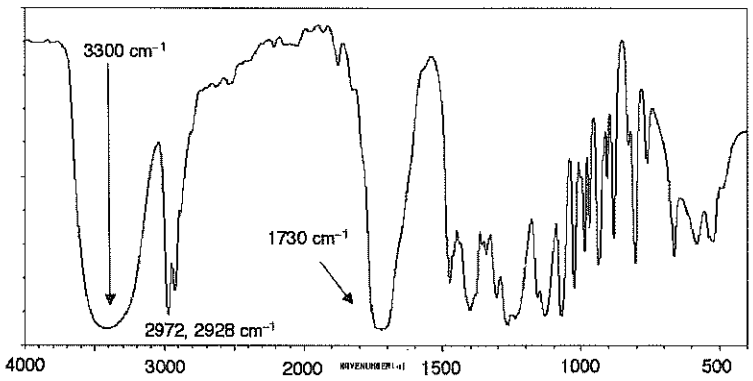
X



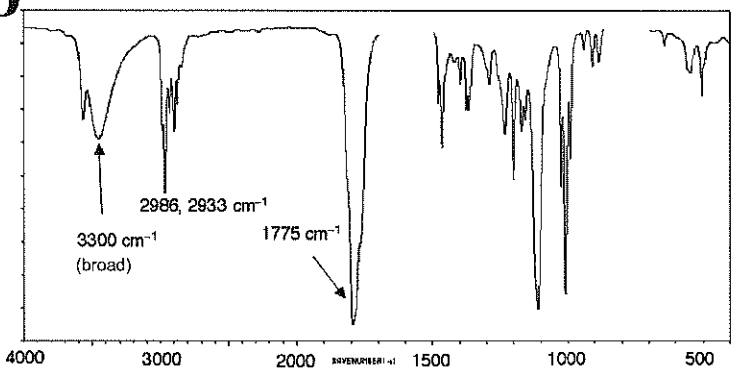
C


E

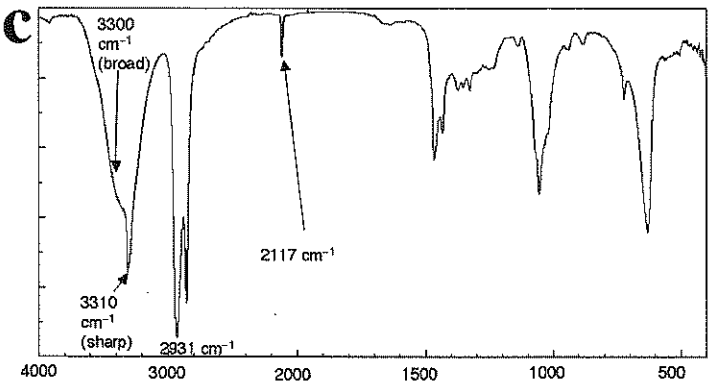
a



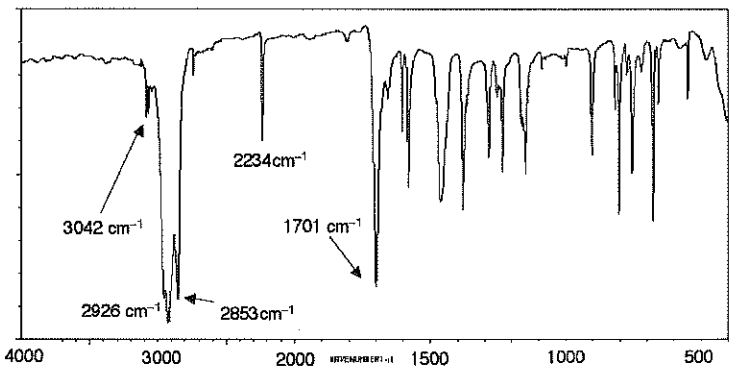
b



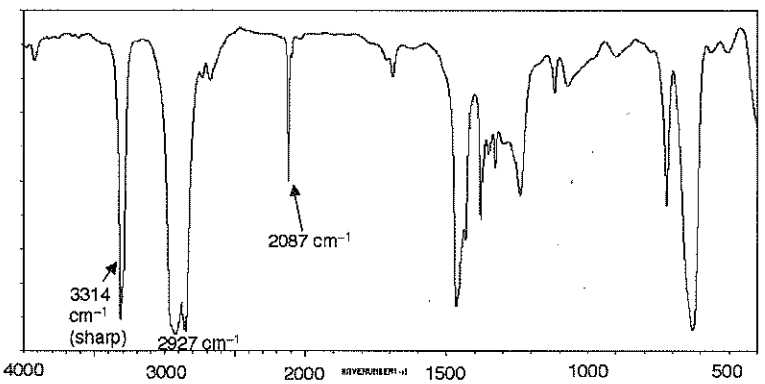
c



d

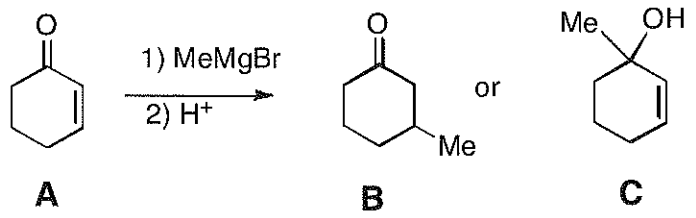


e



2. Reaction of **A** with MeMgBr could lead to either **B** or **C**. Explain how you would use IR spectroscopy to distinguish these compounds

(7 points)



A **B** **C**

For B: expect C=O STRETCH at 1715 cm^{-1}

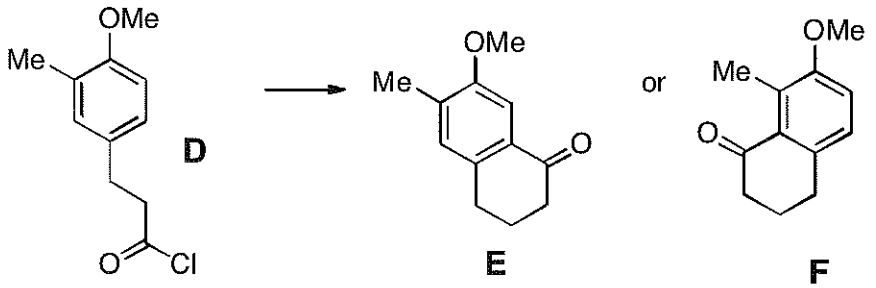
For C: expect C=C STRETCH at ~1650 cm^{-1}

C–H STRETCH at > 3000 cm^{-1}

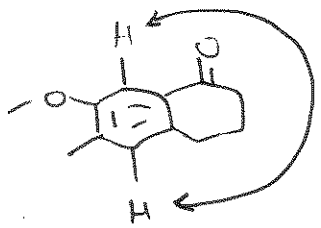
O–H STRETCH: broad peak at ~3300 cm^{-1}

3. $AlCl_3$ catalyzed reaction of **D** could lead to either **E** or **F.** Explain how you would use coupling constants in the ^1H NMR to distinguish these compounds.

(7 points)

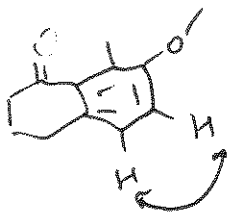


For E:



J_{PARA} ~ 0-1 Hz

For F:



J_{ORTHO} ~ 6-10 Hz

4. Consider the spectroscopic data for compound **1**:

$C_{10}H_{18}O_2$

^{1}H NMR

6.88 (dd, J= 16.0, 6.1 Hz, 1H)
5.83 (d, J = 16.0 Hz, 1H)
4.87 (septet, J=6.8 Hz, 1H)
2.34 (m, 1H)
1.44 (m, 2H)
1.32 (d, J=6.8 Hz, 6H)
1.11 (d, J=6.6 Hz, 3H)
0.90 (t, J=7.0 Hz, 3H)

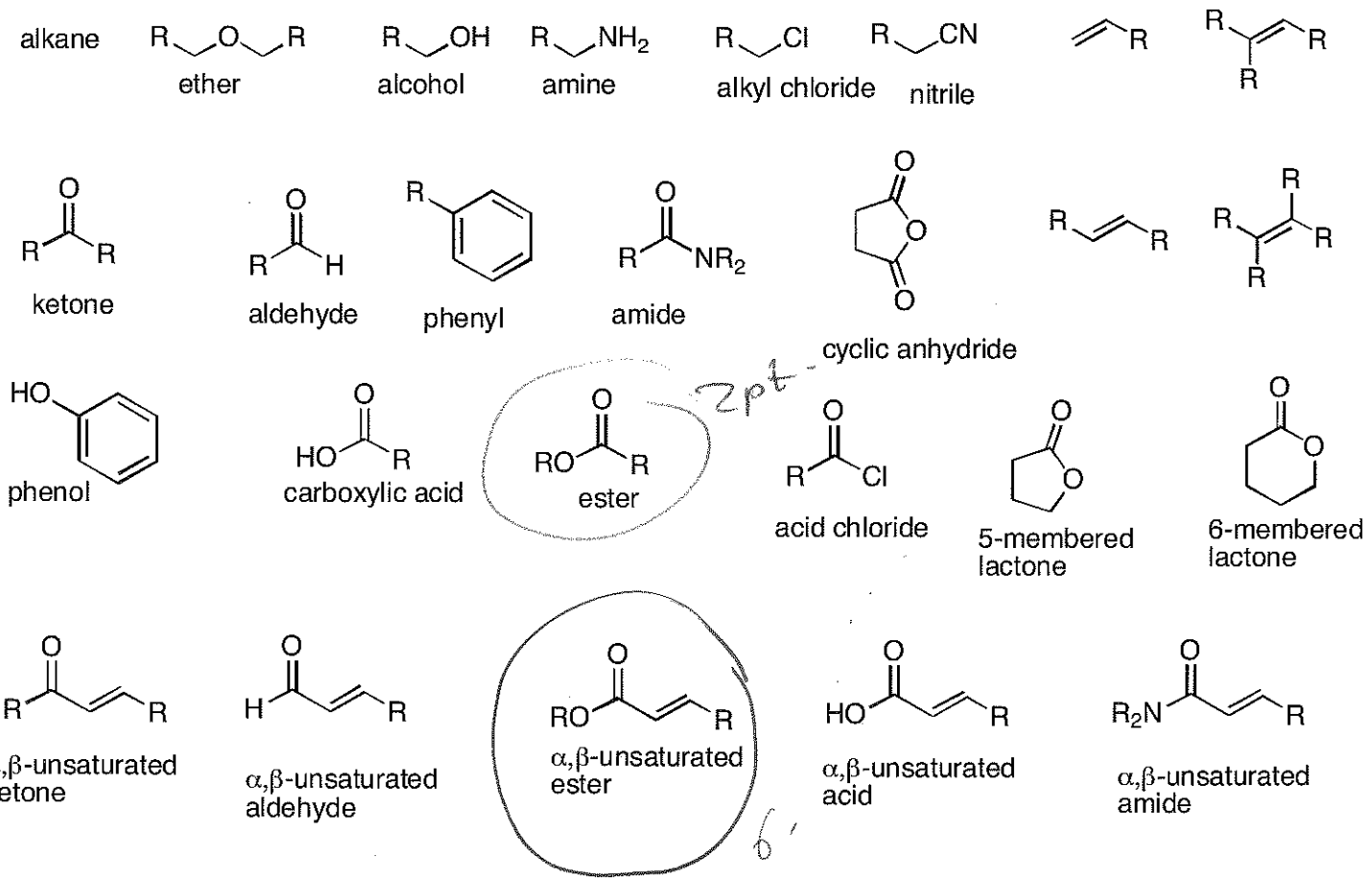
^{13}C NMR

168.0, s
155.8, d
120.3, d
70.8, d
38.2, d
29.5, t
21.7, q (2 carbons)
20.0, q
11.7, q

IR: 1720 cm^{-1}

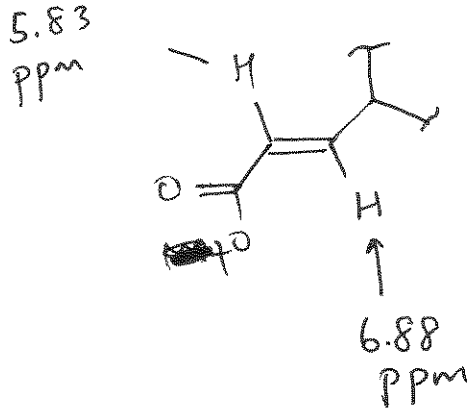
a) Circle the functional group that is associated with (6 points)

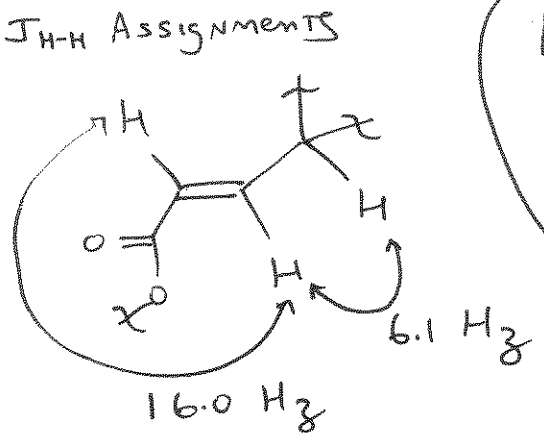
(i) IR: 1720 cm^{-1}

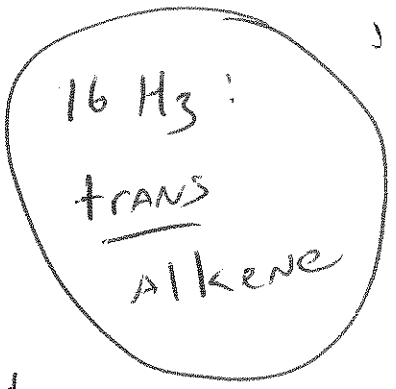


b. Assign the following coupling constants
For your answer, draw the substructure of your product, and specify any stereochemical information that is indicated by the coupling constants: (7 points)

6.88 (dd, J= 16.0, 6.1 Hz, 1H)
5.83 (d, J = 16.0 Hz, 1H)

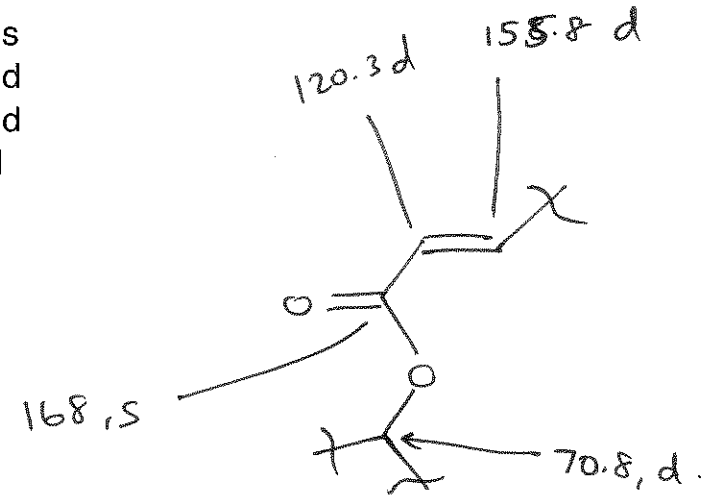




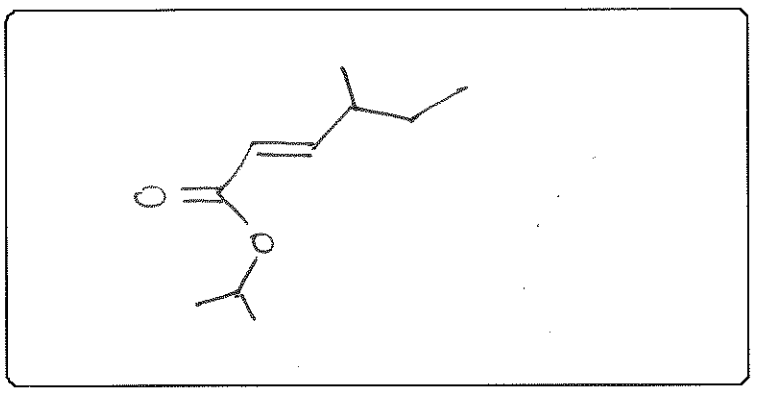


c. Assign the substructure associated with the following ^{13}C NMR resonances (7 points)

168.0, s
155.8, d
120.3, d
70.8, d



d) draw the structure of the product (no partial credit) (10 points)



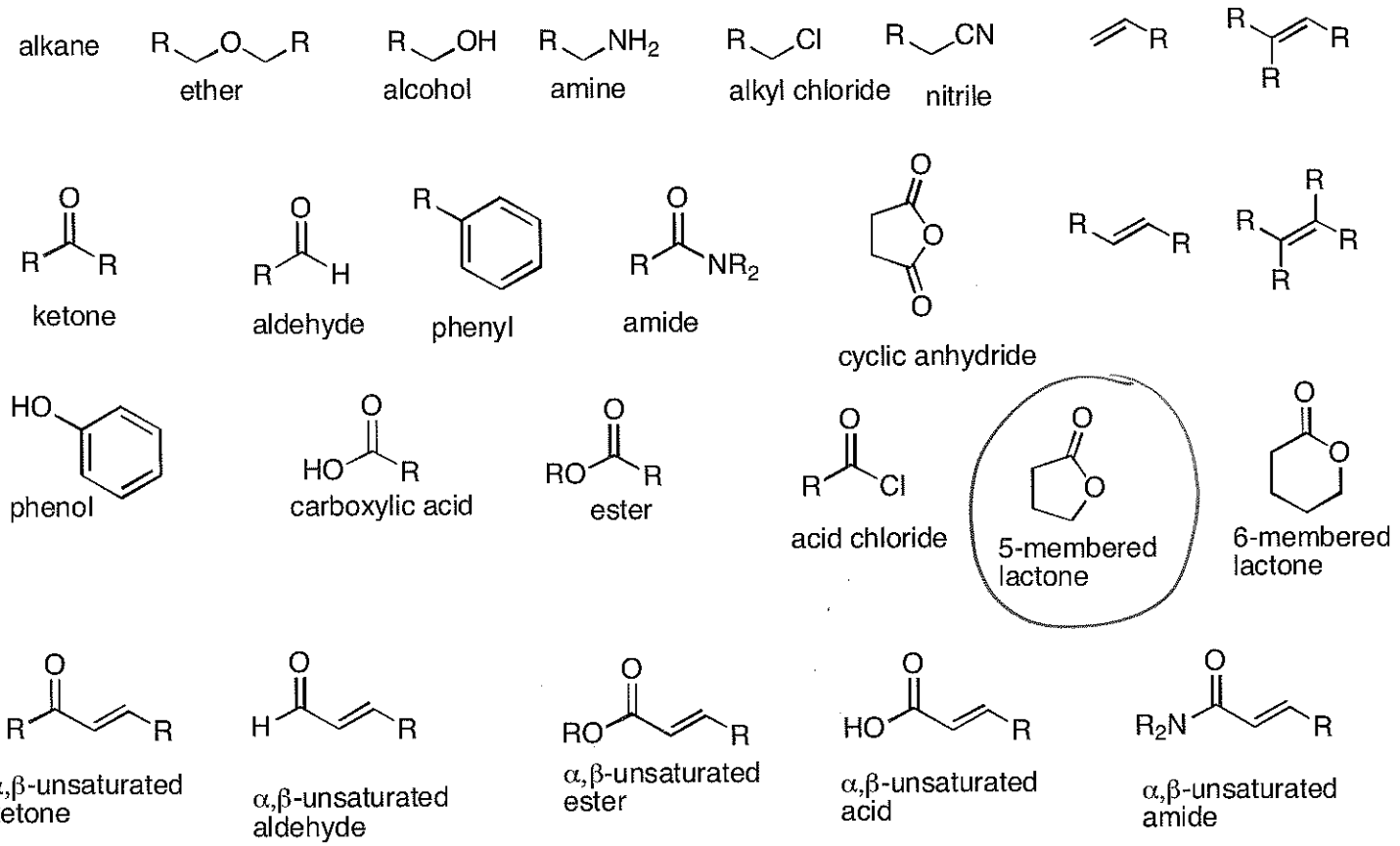
5. Consider the spectroscopic data for compound **2**:

$C_{11}H_{12}O_3$

^{1}H NMR	**^{13}C NMR**	**IR:**
		1770 cm^{-1}
7.16 (d, J = 8.4 Hz, 2H)	176.8, s	
6.90 (d, J = 8.4 Hz, 2H)	159.3, s	
4.64 (dd, J = 9.1, 7.1 Hz, 1H)	140.1, s	
4.23 (dd, J = 9.1, 6.8 Hz, 1H)	128.0, d (2 carbons)	
3.81 (s, 3H)	114.7, d (2 carbons)	
3.39 (m, 1H)	74.5, t	
2.90 (dd, J = 7.7, 17.4 Hz, 1H)	55.6, q	
2.63 (dd, J = 7.4, 17.4 Hz, 1H)	40.7, t	
	36.1, d	

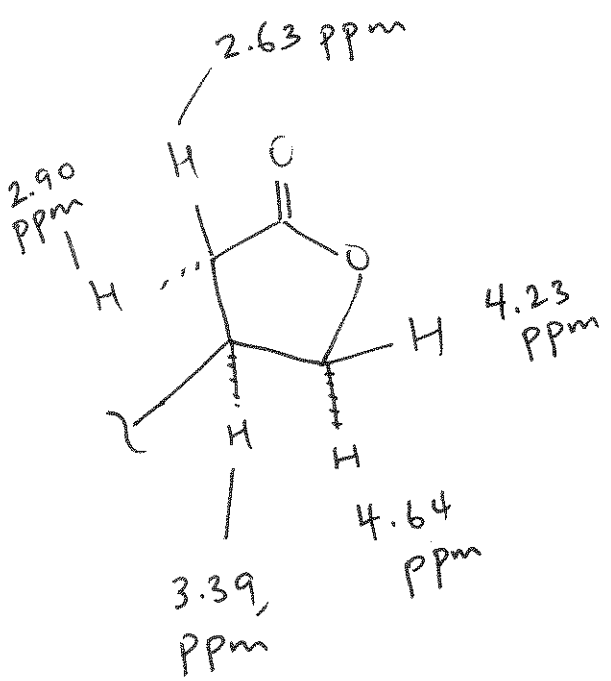
a) Circle the functional group that is associated with (6 points)

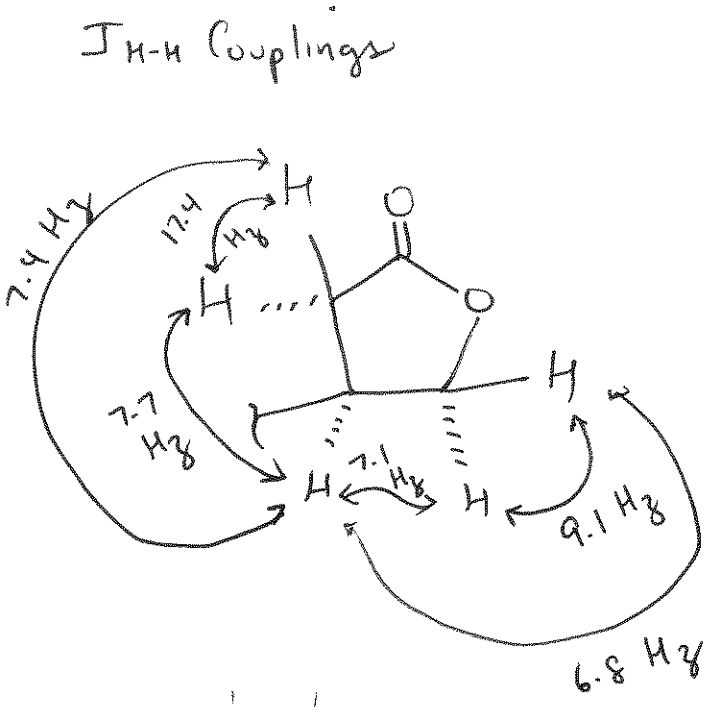
(i) IR: 1770 cm^{-1}



b. Assign the following coupling constants and chemical shifts (14 points)
For your answer, draw the substructure of your product, and specify any stereochemical information that is indicated by the coupling constants:

4.64 (dd, J = 9.1, 7.1 Hz, 1H)
4.23 (dd, J = 9.1, 6.8 Hz, 1H)
3.39 (m, 1H)
2.90 (dd, J = 7.7, 17.4 Hz, 1H)
2.63 (dd, J = 7.4, 17.4 Hz, 1H)



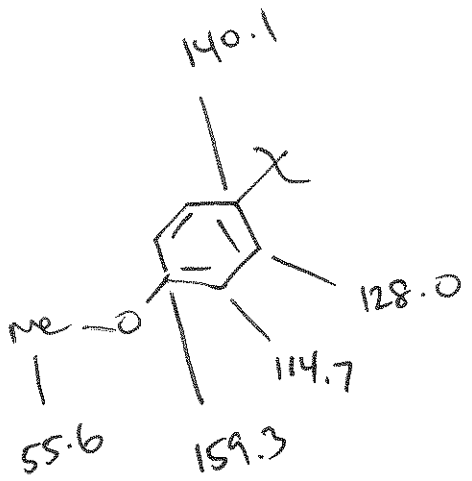


P.6

(8 points)

c. Assign the substructure associated with the following ^{13}C NMR resonances

159.3, s
140.1, s
128.0, d (2 carbons)
114.7, d (2 carbons)
55.6, q



d) draw the structure of the product (no partial credit) (13 points)