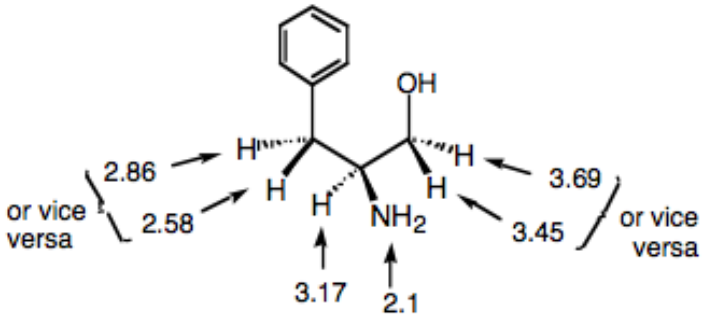
Chem 334, Exam 1
Professor Fox
Spring 2010

Your Name_____

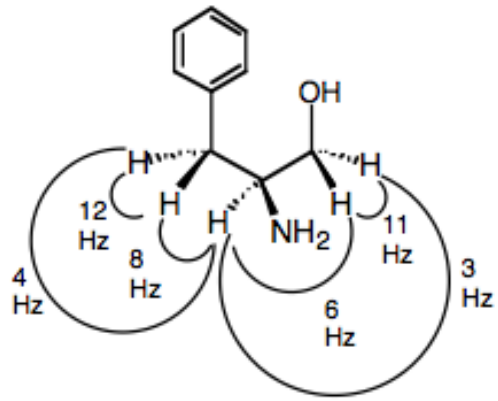
Open note, open book

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

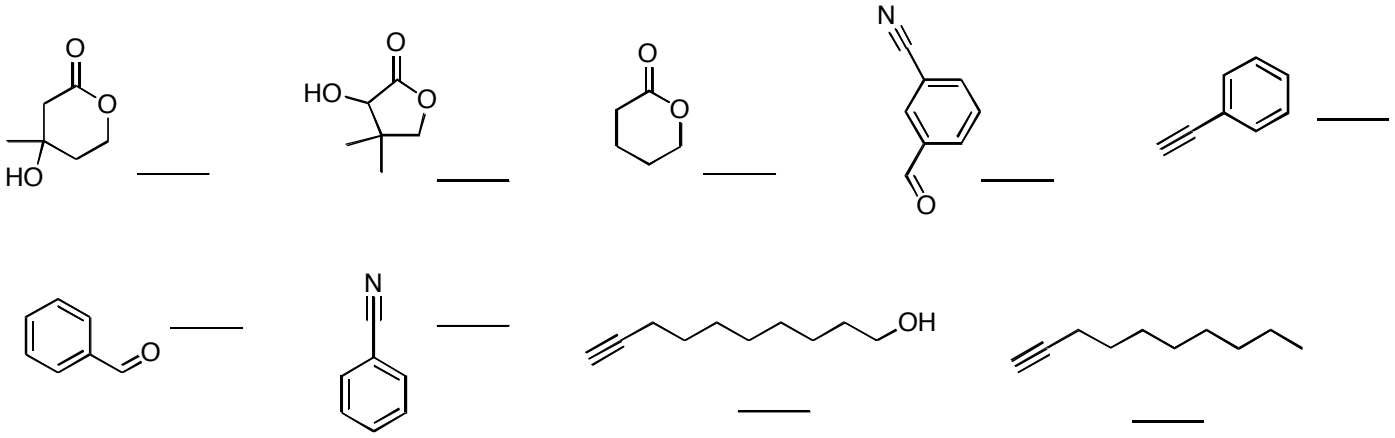
**$^1$H assignments**



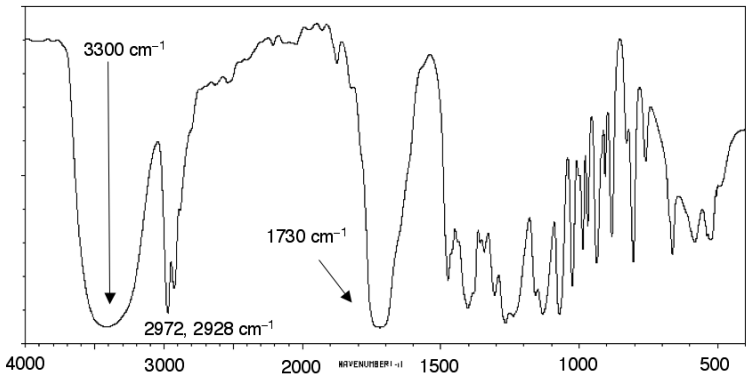

**$J_{H\text{-}H}$ assignments**



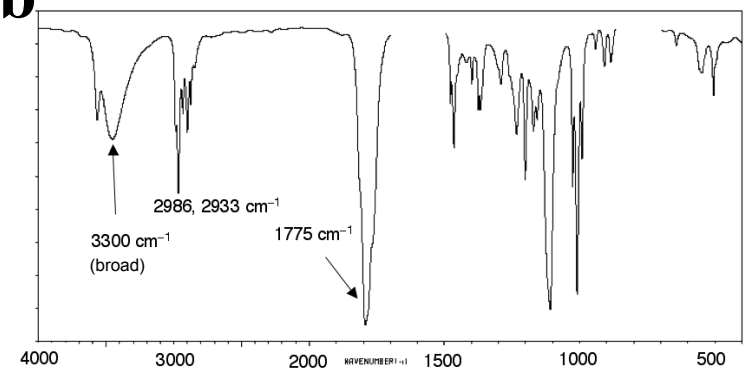
1. Match the following to their IR spectra. (15 points) (not all compounds have a match). Place an X next to compounds without a match



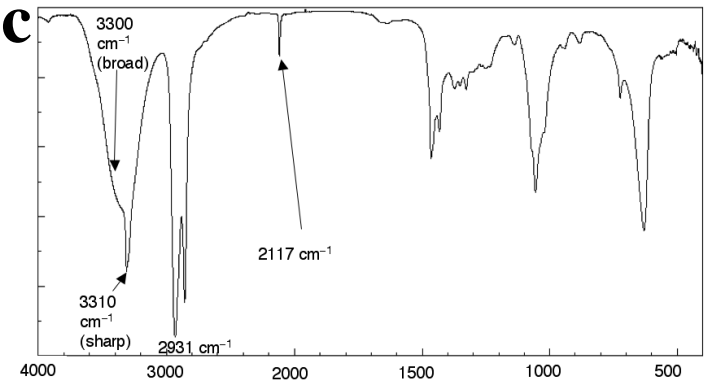

**a**



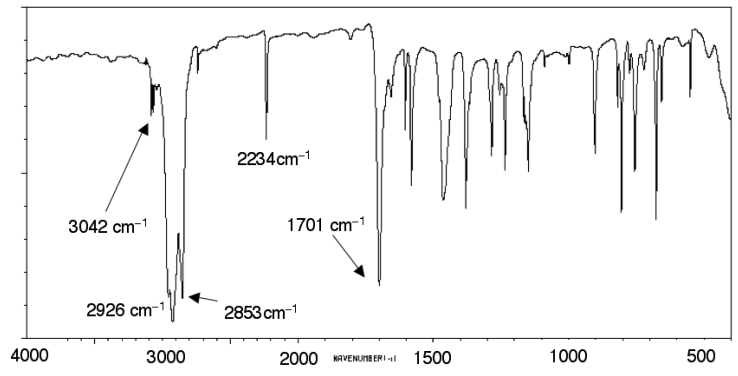

**b**



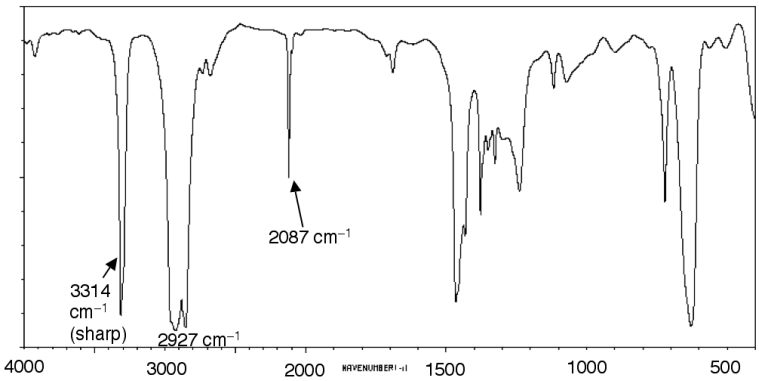

**c**




**d**

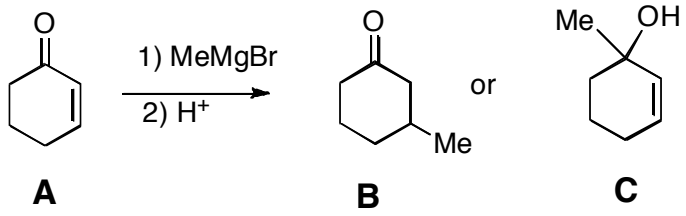



**e**



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

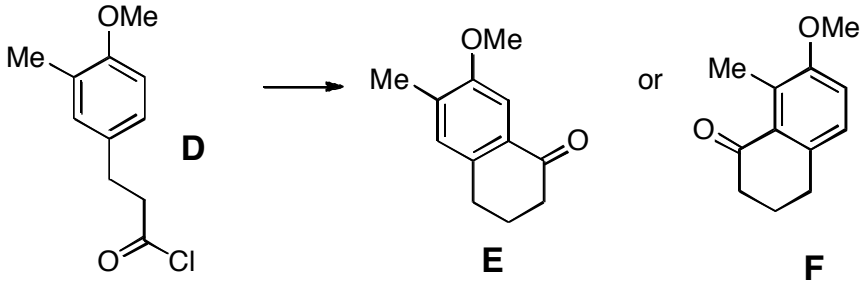
(7 points)




**A** **B** **C**

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)




**D** **E** **F**

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)

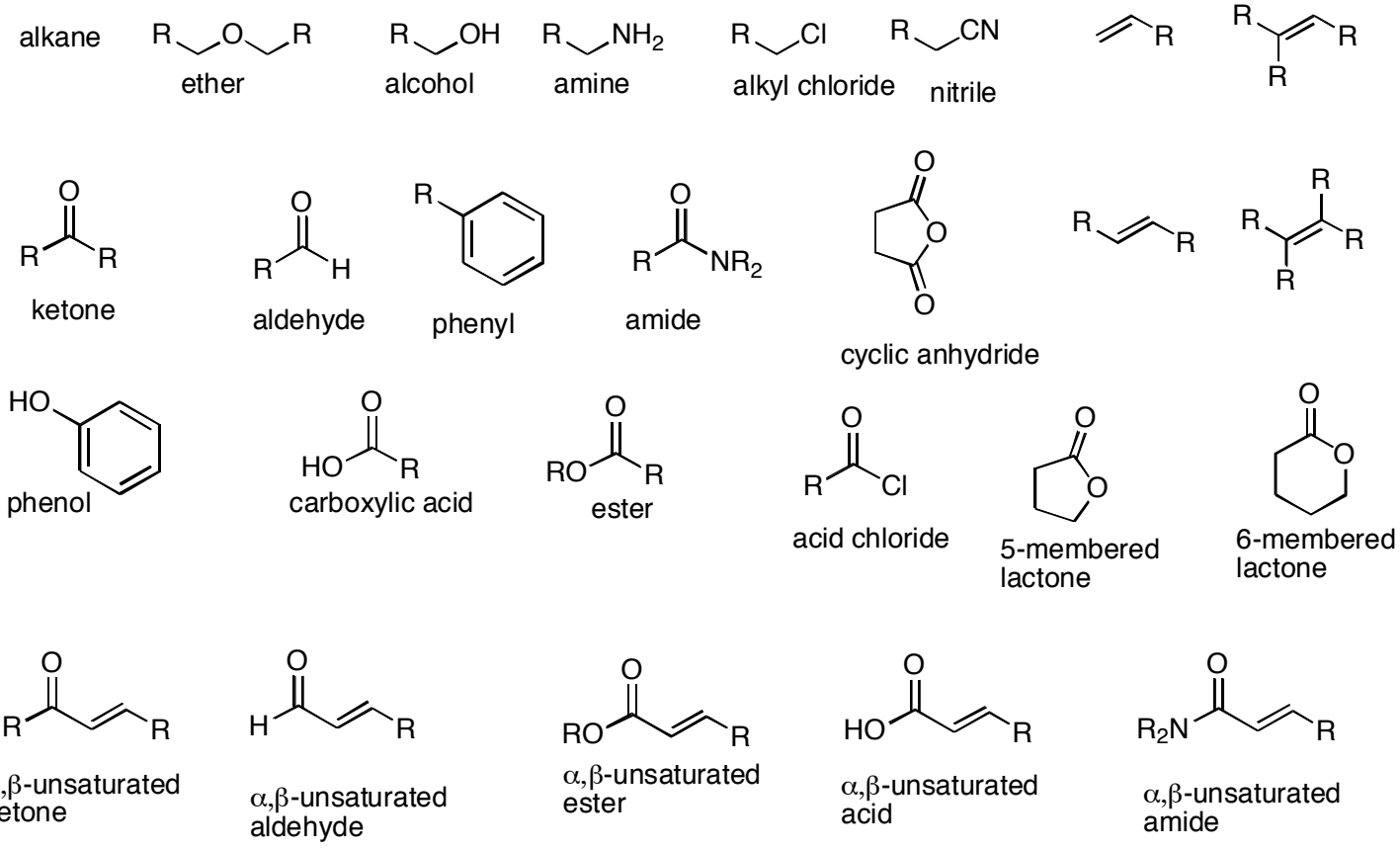
**$^{13}$C NMR**

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)

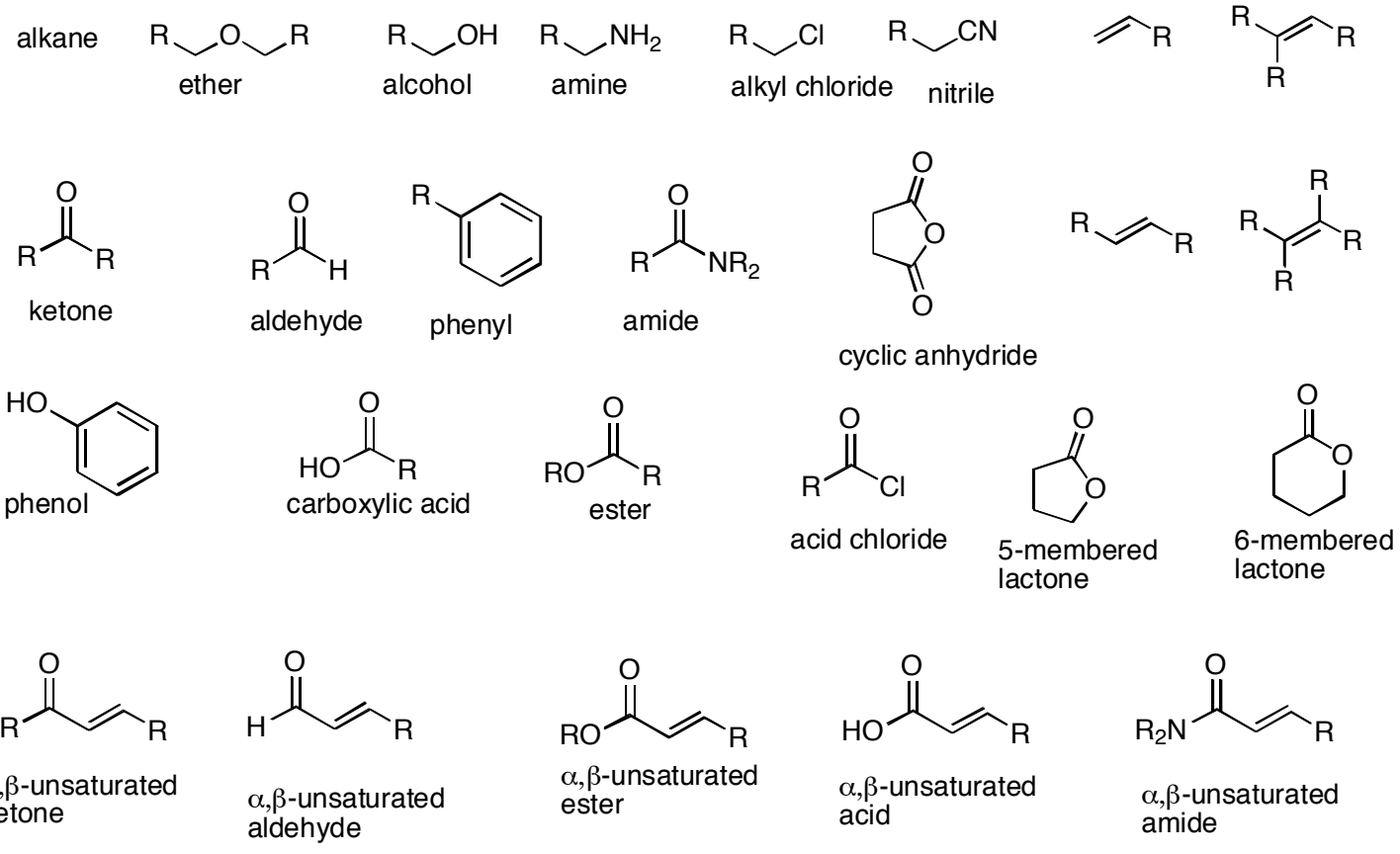
5. Consider the spectroscopic data for compound **2**:

**$C_{11}H_{12}O_3$**

| **$^1$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:

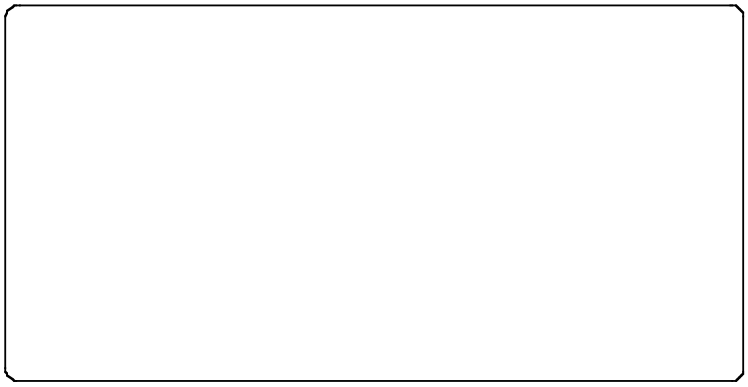
4.64 (dd, *J* = 9.1, 7.1 Hz, 1H)
4.23 (dd, *J* = 9.1, 6.8 Hz, 1H)
3.39 (m, 1H)
2.90 (dd, *J* = 7.7, 17.4 Hz, 1H)
2.63 (dd, *J* = 7.4, 17.4 Hz, 1H)

(8 points)

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

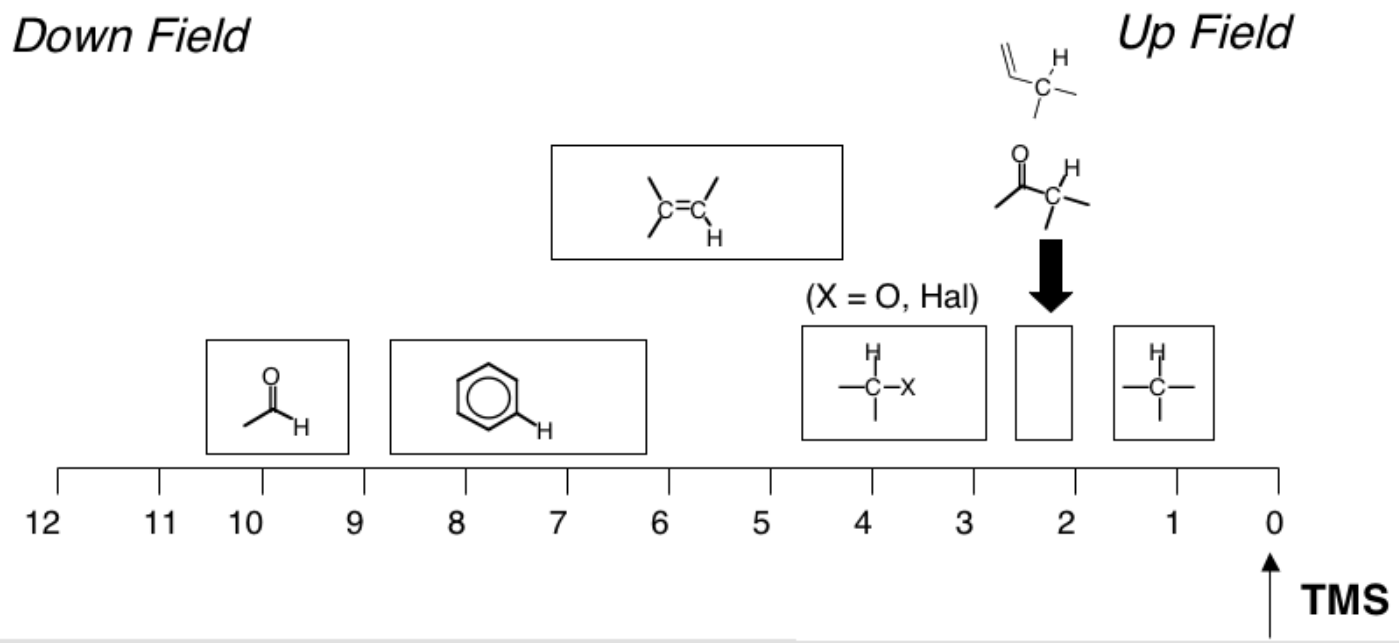
159.3, s
140.1, s
128.0, d (2 carbons)
114.7, d (2 carbons)
55.6, q

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

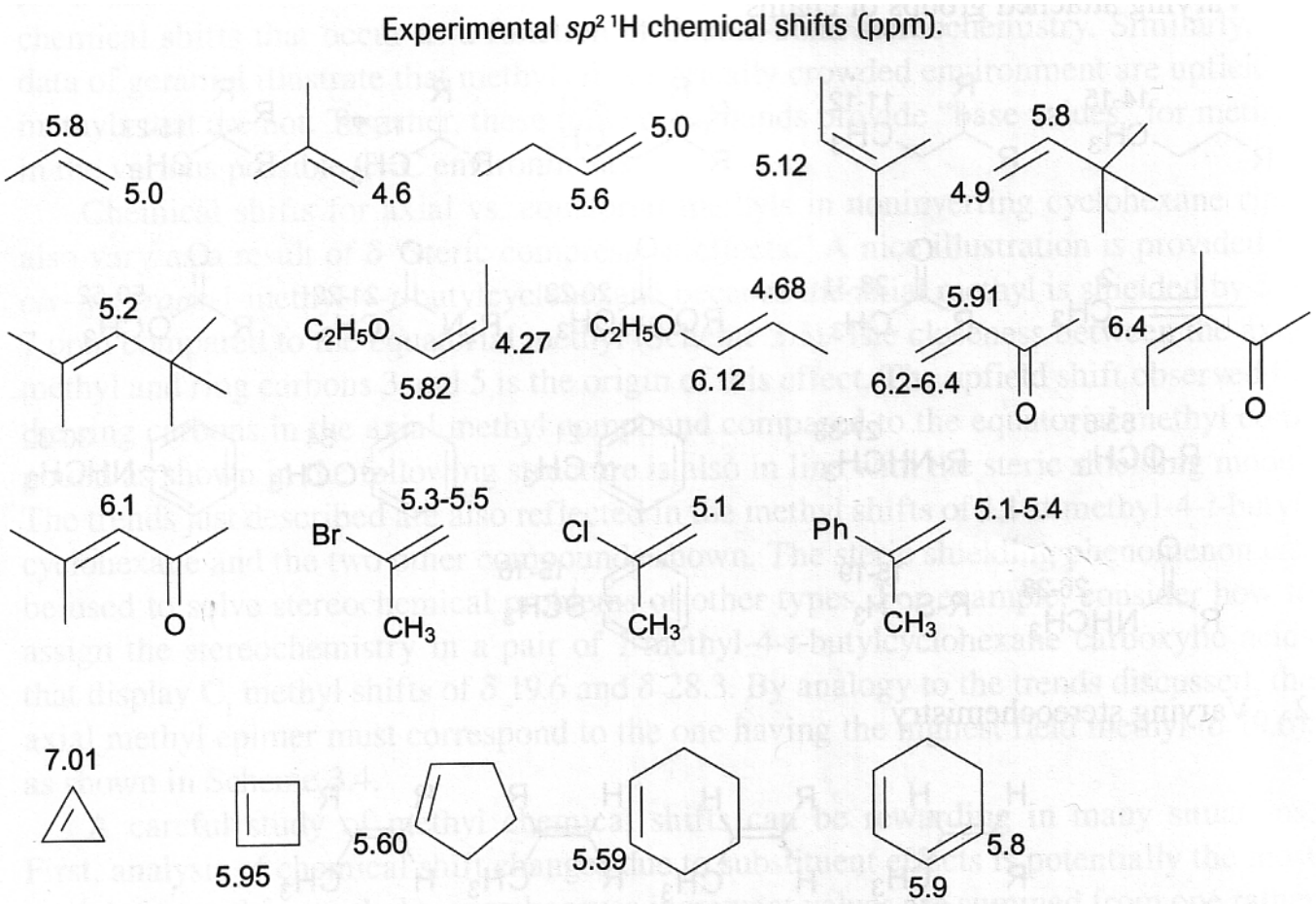


Overview of *typical* $^1$H NMR shifts

**Note:** alkene region modified from earlier handout

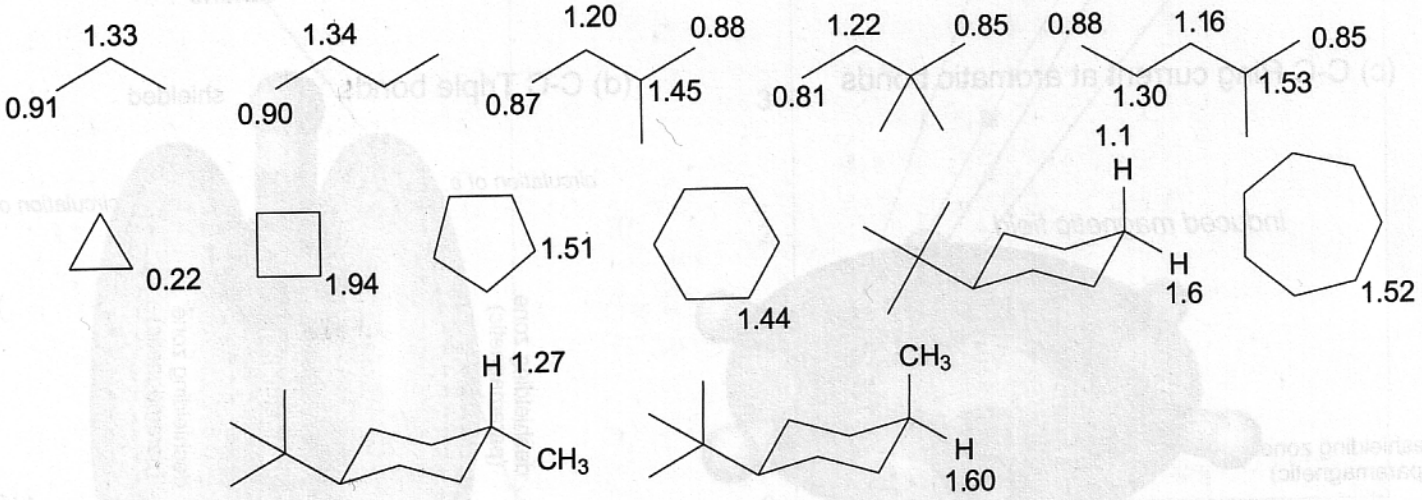



# $^1$H NMR Tables

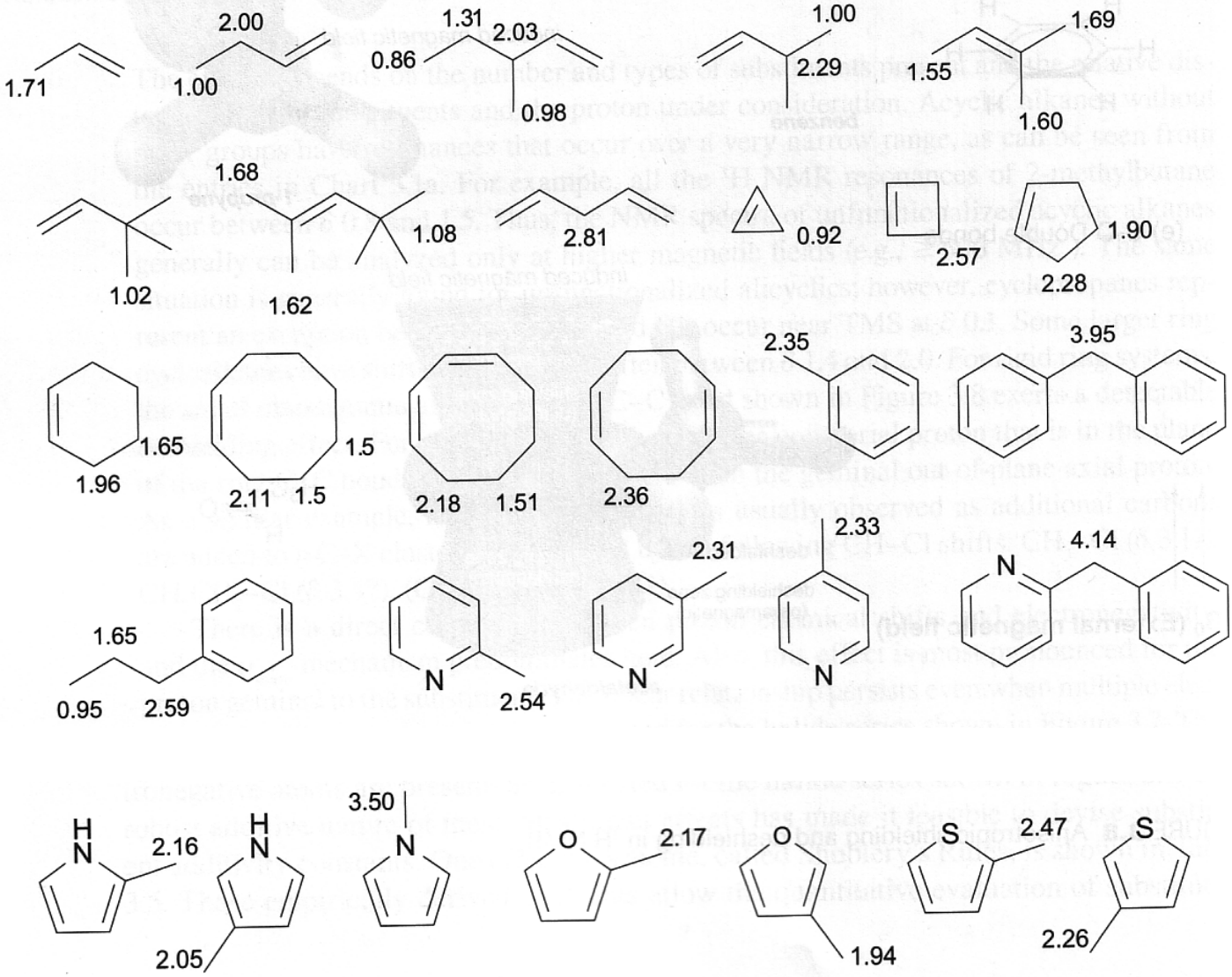


# $^1$H NMR Tables

## Alkanes



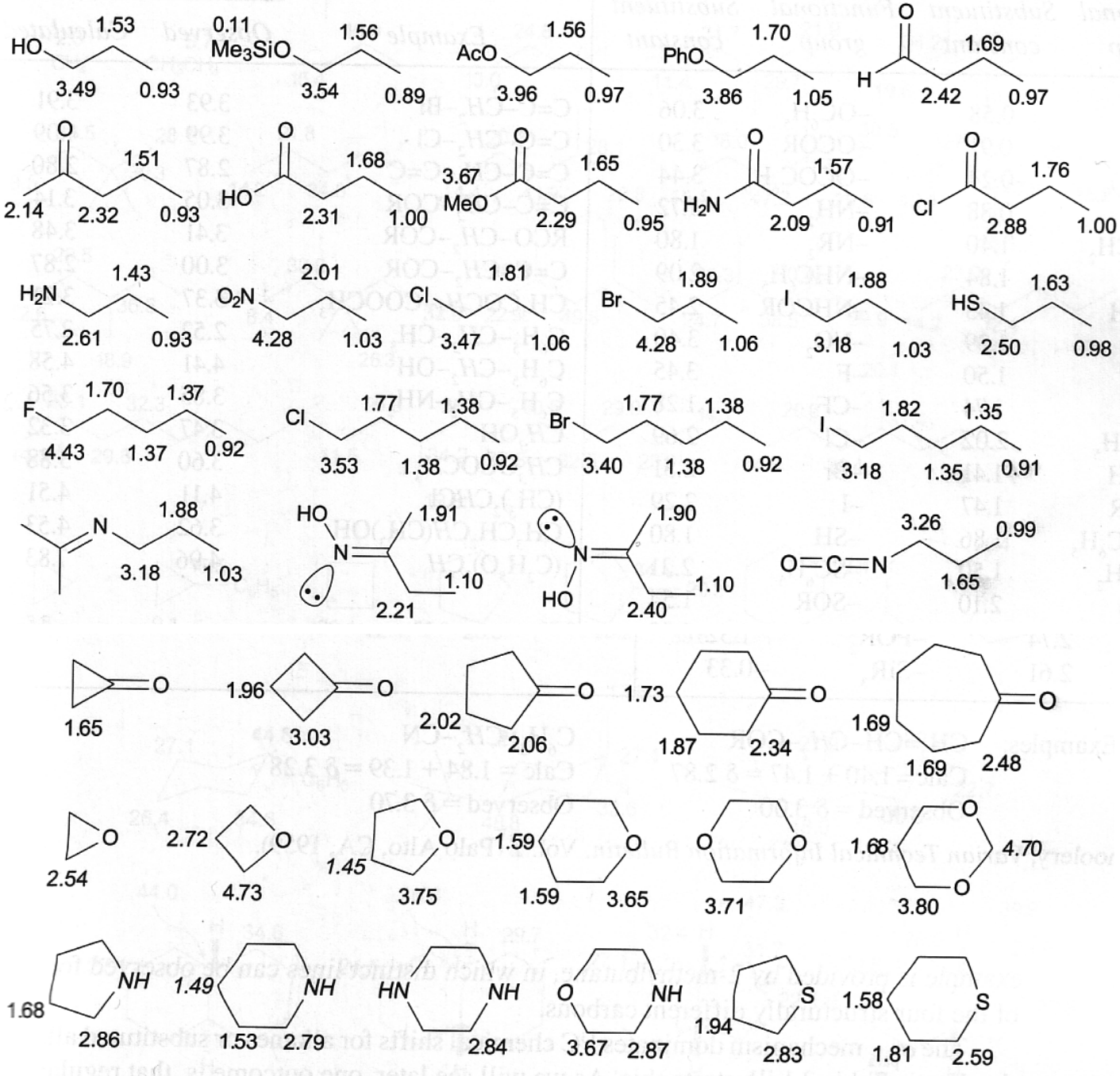

## Substituted Alkanes



# $^1$H NMR Tables

Experimental $sp^3$ $^1$H chemical shifts (ppm) (*cont.*).

## Functionalized Alkanes




## Substituted Alkynes and C≡N