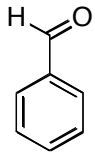
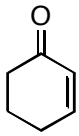
for answers: see Chem 334, 2008, exam 1: http://www.udel.edu/chem/fox/chem334Spring2009.html

2. Match the following NMR spectra with one of the following substances. Write you answer in the box along side the spectrum

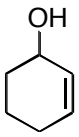
(16 points)



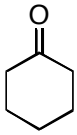
A



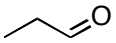
B



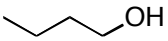
C



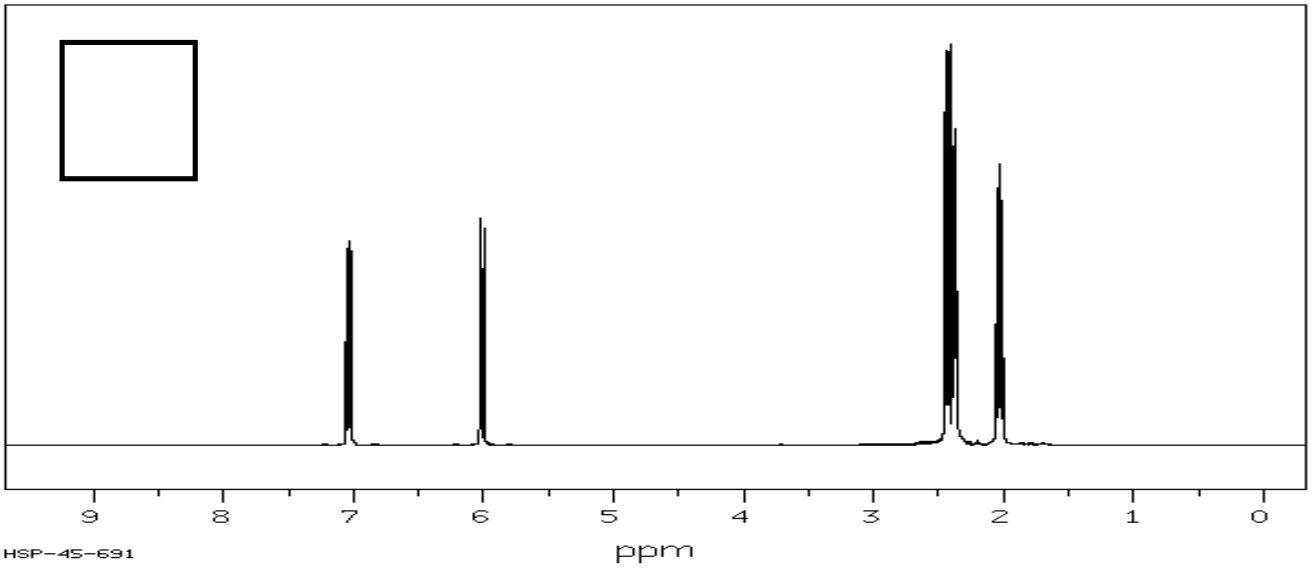
D

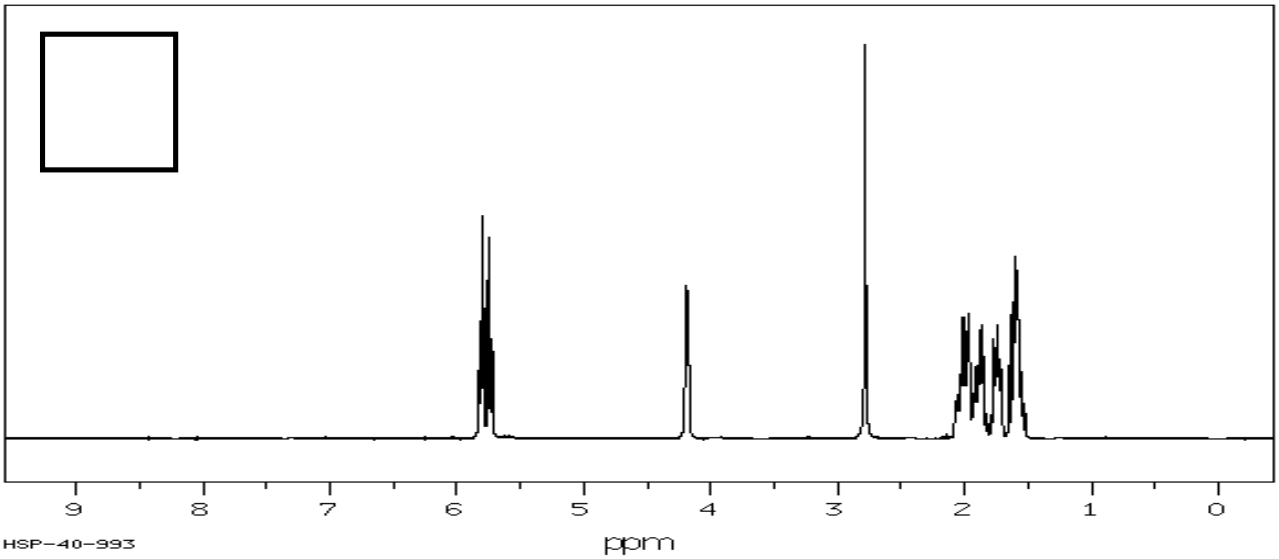


E



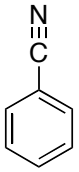
F



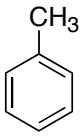


for answers: see Chem 334, 2009, exam 2: http://www.udel.edu/chem/fox/chem334Spring2009.html

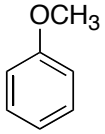
1. Match the following compounds with their ^{13}C NMR spectra. Note: only chemical shift data is given [multiplicities (s,d,t,q) are not needed to solve this problem]



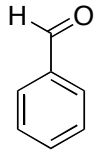
A



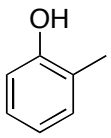
B



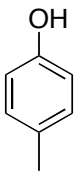
C



D

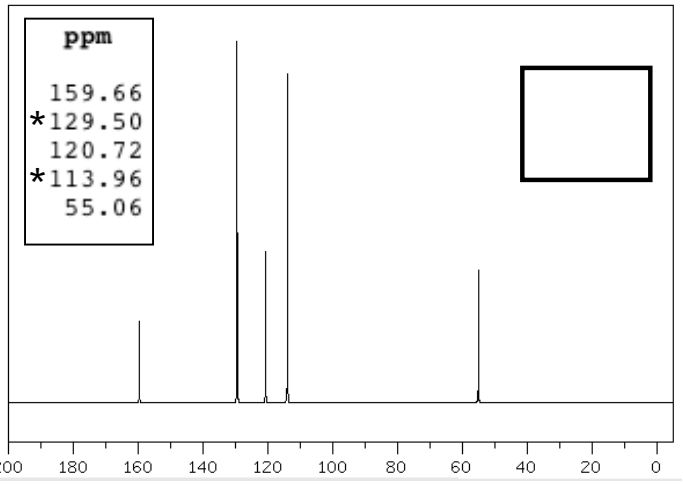


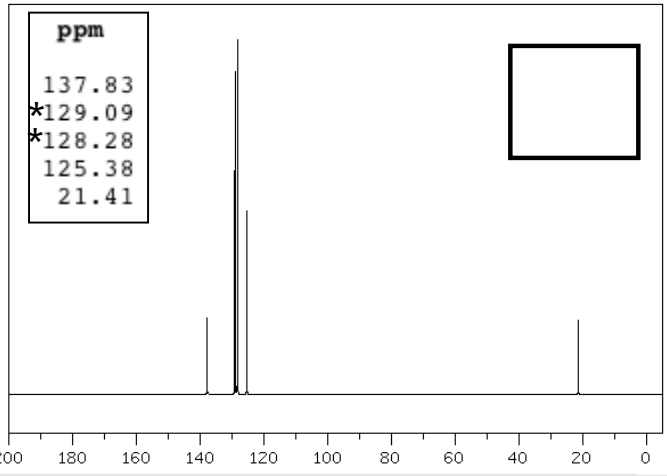
E

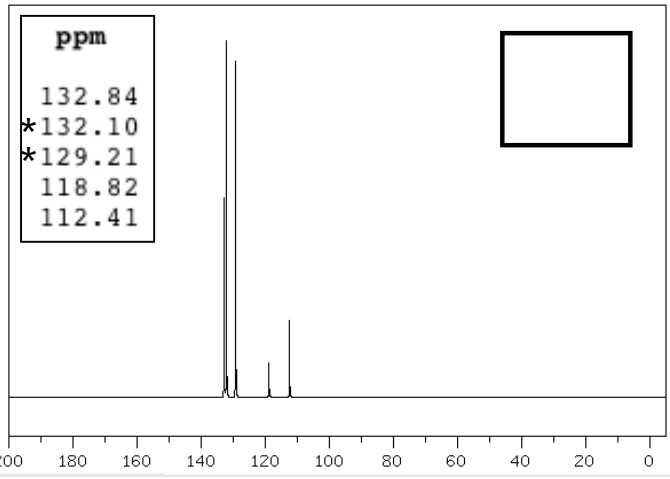


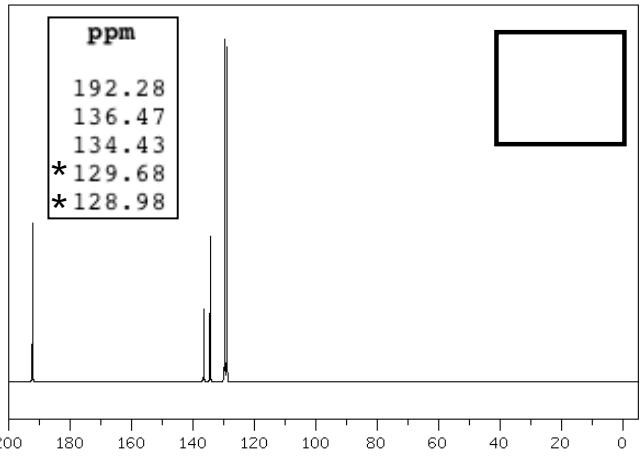
F

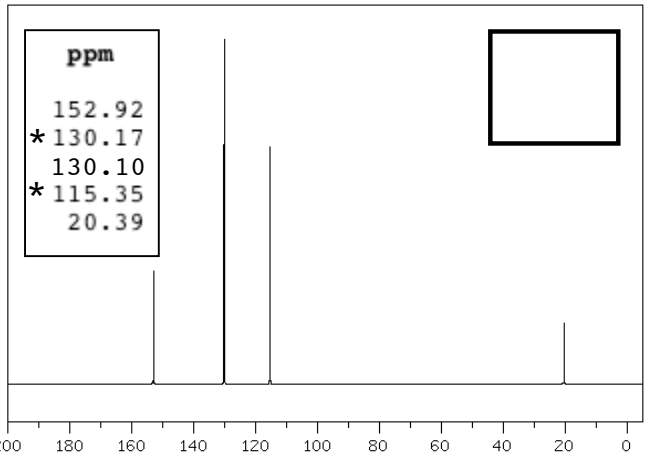
Note: * = 2 carbons

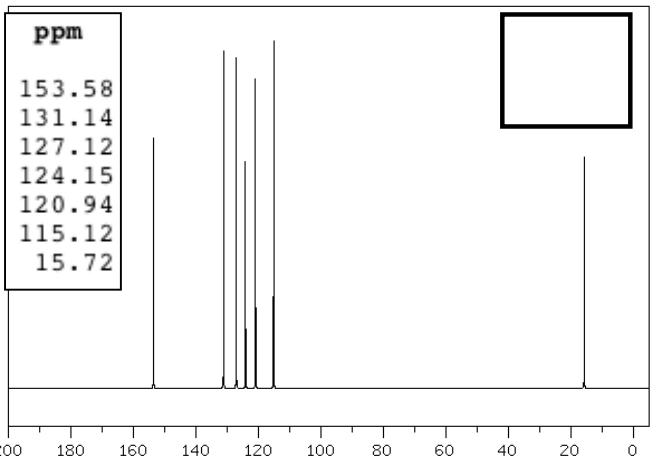






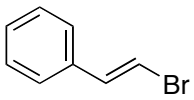


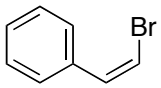




for answers: see Chem 334, 2009, exam 2: http://www.udel.edu/chem/fox/chem334Spring2009.html

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





for answers: see Chem 334, 2007, exam 1: http://www.udel.edu/chem/fox/chem334Spring2009.html

3. Elucidate the following structure

$C_{15}H_{11}BrO_2$

^{1}H NMR

7.93 (d, J = 7.5 Hz, 1H),
7.58 (d, J=7.6 Hz, 2H),
7.52 (t, J = 8.0 Hz, 1H)
7.36 (d, J=7.6 Hz, 2H),
7.09-7.05 (m, 2H)
5.45 (dd, J = 13.3, 2.6Hz, 1H)
3.00 (dd, J = 16.8, 13.3 Hz, 1H)
2.88 (dd, J = 16.8, 2.6 Hz, 1H)

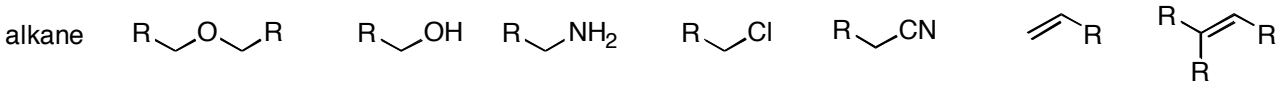
^{13}C NMR

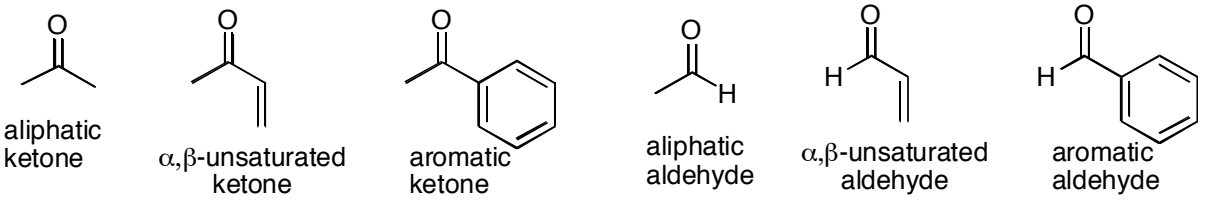
196 (s)
162 (s)
138 (s)
136 (d)
132 (d) (2 carbons)
128 (d) (2 carbons)
127 (d)
123 (s)
122 (s)
121 (d)
118 (d)
79 (d)
44 (t)

IR: 1692, 1605, 1465 cm^{-1}

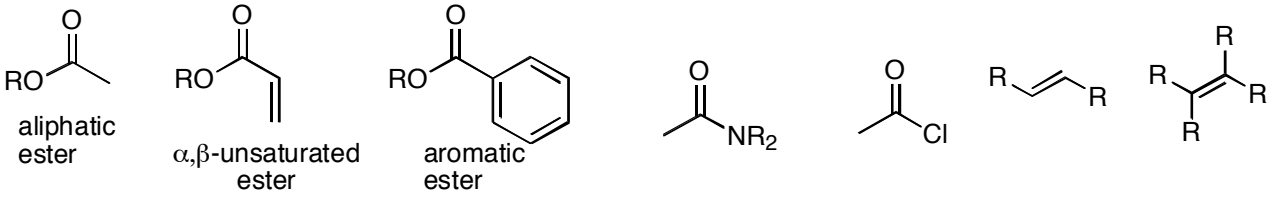
a) Circle the functional group that is associated with

(i) IR: 1692 cm^{-1} (9 points)





aliphatic ketone | α,β-unsaturated ketone | aromatic ketone | aliphatic aldehyde | α,β-unsaturated aldehyde | aromatic aldehyde



aliphatic ester | α,β-unsaturated ester | aromatic ester

3. Elucidate the following structure

$C_{15}H_{11}BrO_2$

continued

^{1}H NMR

7.93 (d, J = 7.5 Hz, 1H),
7.58 (d, J=7.6 Hz, 2H),
7.52 (t, J = 8.0 Hz, 1H)
7.36 (d, J=7.6 Hz, 2H),
7.09-7.05 (m, 2H)
5.45 (dd, J = 13.3, 2.6Hz, 1H)
3.00 (dd, J = 16.8, 13.3 Hz, 1H)
2.88 (dd, J = 16.8, 2.6 Hz, 1H)

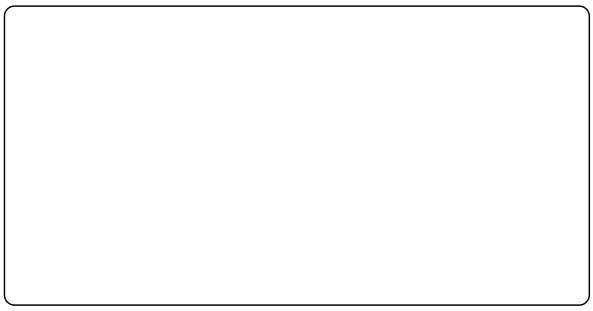
^{13}C NMR

196 (s)
162 (s)
138 (s)
136 (d)
132 (d) (2 carbons)
128 (d) (2 carbons)
127 (d)
123 (s)
122 (s)
121 (d)
118 (d)
79 (d)
44 (t)

IR: 1692, 1605, 1465 cm^{-1}

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

(25 points)



c. Assign the following coupling constants: (20 points)

5.45 (dd, J = 13.3, 2.6Hz, 1H)
3.00 (dd, J = 16.8, 13.3 Hz, 1H)
2.88 (dd, J = 16.8, 2.6 Hz, 1H)

2. Elucidate the following structure

$C_{11}H_{13}NO_3$

^{13}C NMR

208.2 (s)
148.5 (s)
135.4 (d)
135.2 (s)
129.5 (d)
124.4 (d)
122.0 (d)
48.4 (d)
31.0 (t)
15.8 (q)
7.9 (q)

^{1}H NMR

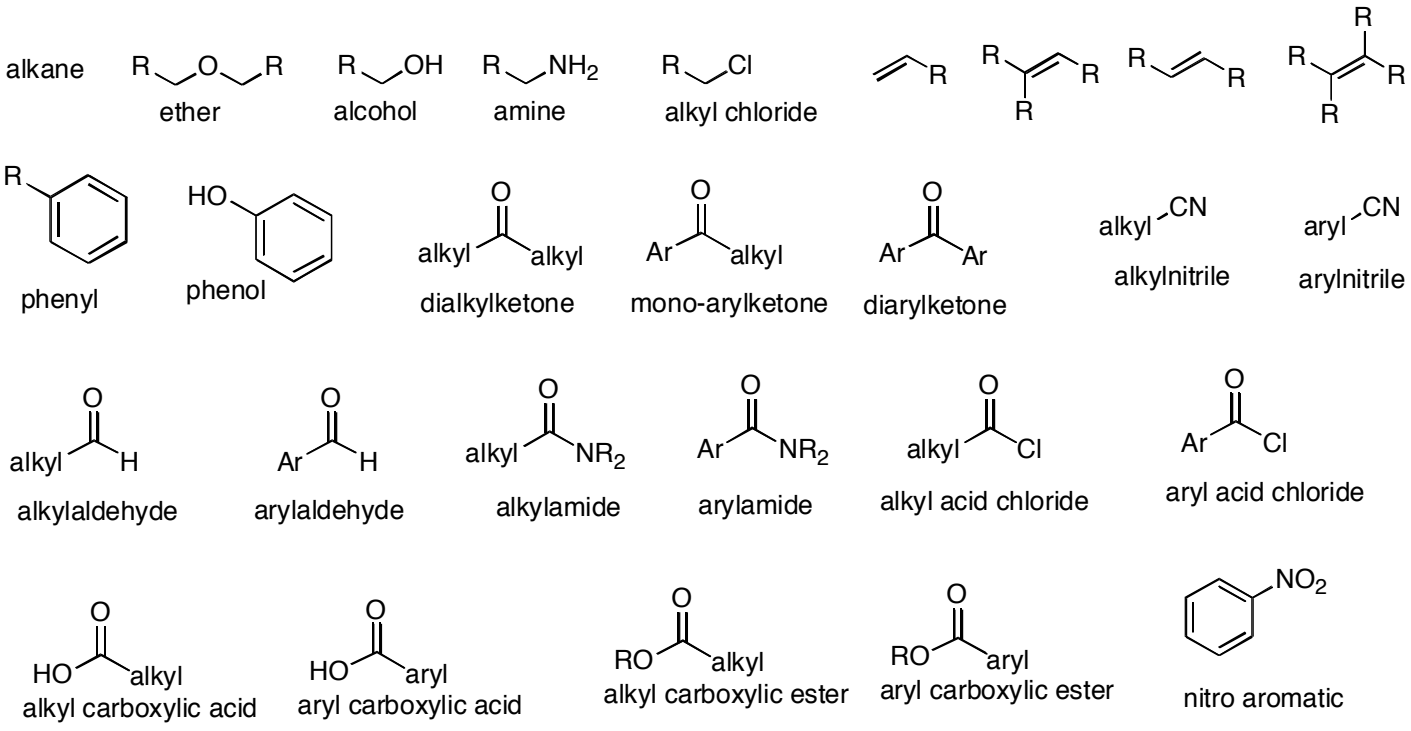
8.05 (t, J=2.1 Hz, 1H)
8.01 (dt, J=7.9, 2.1 Hz, 1H)
7.51 (dt, J=7.9, 2.1 Hz, 1H)
7.47 (t, J=7.9 Hz, 1H)
3.81 (q, J=6.8 Hz, 1H)
2.49 (m, 2H)
1.44 (d, J=6.8 Hz, 3H)
1.06 (t, J=7.0 Hz, 3H)

IR:
1715, 1520, 1350 cm^{-1}

a) Circle the functional group that is associated with

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

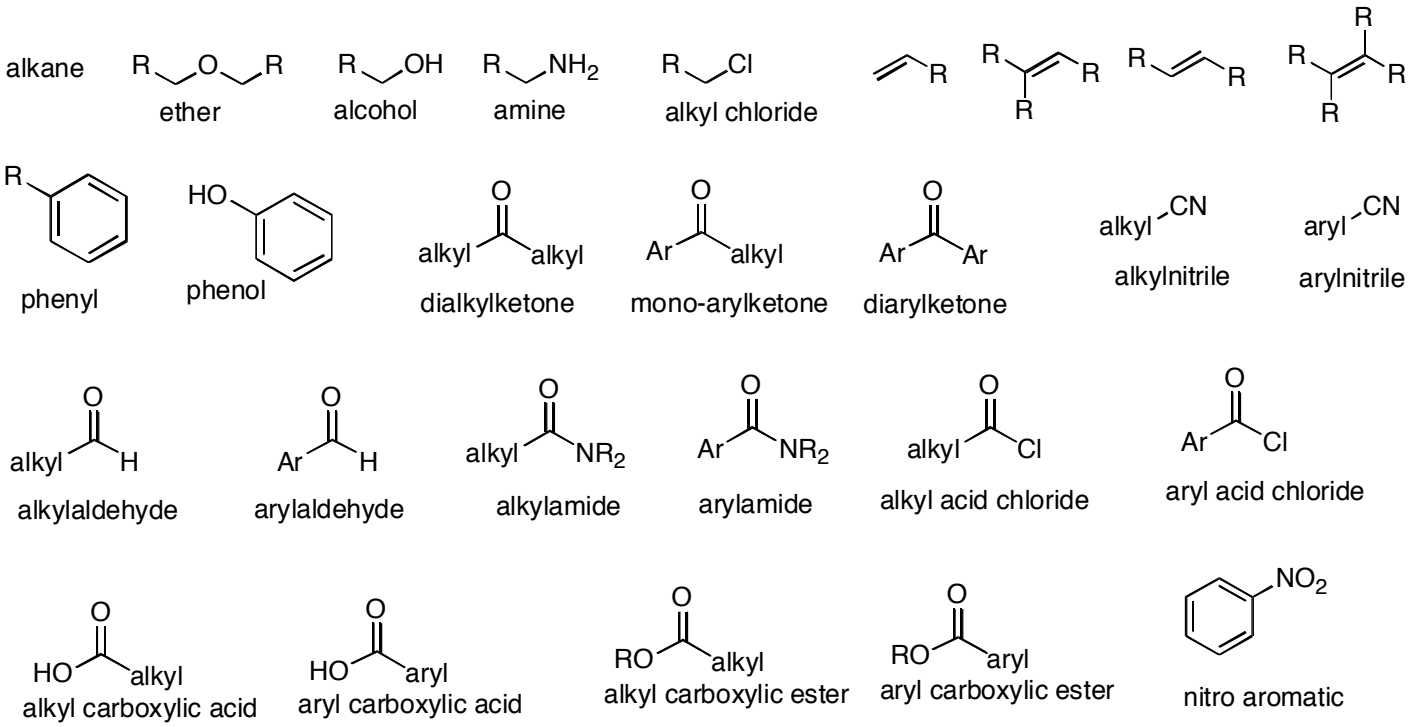
(i) IR: 1520 and 1350 cm^{-1} (both peaks are associated with one functional group)



b) Circle the functional group that is associated with

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

(i) IR: 1715 cm^{-1} (both peaks are associated with one 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:

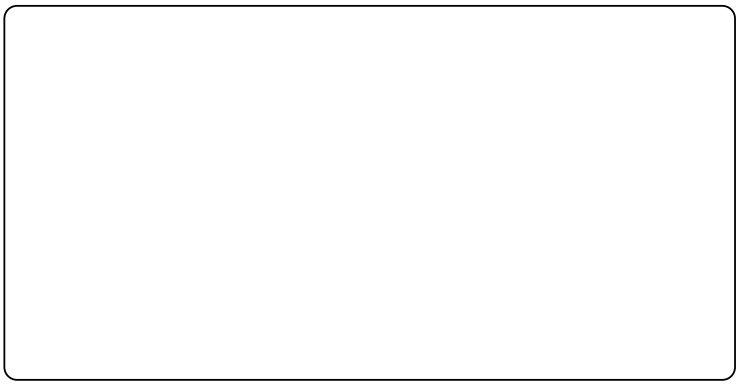
3.81 (q, J=6.8 Hz, 1H)
1.44 (d, J=6.8 Hz, 3H)

2 Elucidate the following structure (continued)

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

8.05 (t, J=2.1 Hz, 1H)
8.01 (dt, J=7.9, 2.1 Hz, 1H)
7.51 (dt, J=7.9, 2.1 Hz, 1H)
7.47 (t, J=7.9 Hz, 1H)

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



for answers: see Chem 334, 2007, exam 2: http://www.udel.edu/chem/fox/chem334Spring2009.html

5. Elucidate the following structure

AD: $C_{13}H_{18}O_3$

7.86 ppm (d, J=8.0 Hz, 2H)
6.88 ppm (d, J=8.0 Hz, 2H)
3.86 ppm (m, 1H)
3.91 (s, 3H)
1.67 (m, 2H)
1.43 (d, J=7.0 Hz, 3H)
1.33 (m, 2H)
0.96 (t, J=6.9 Hz, 3H)

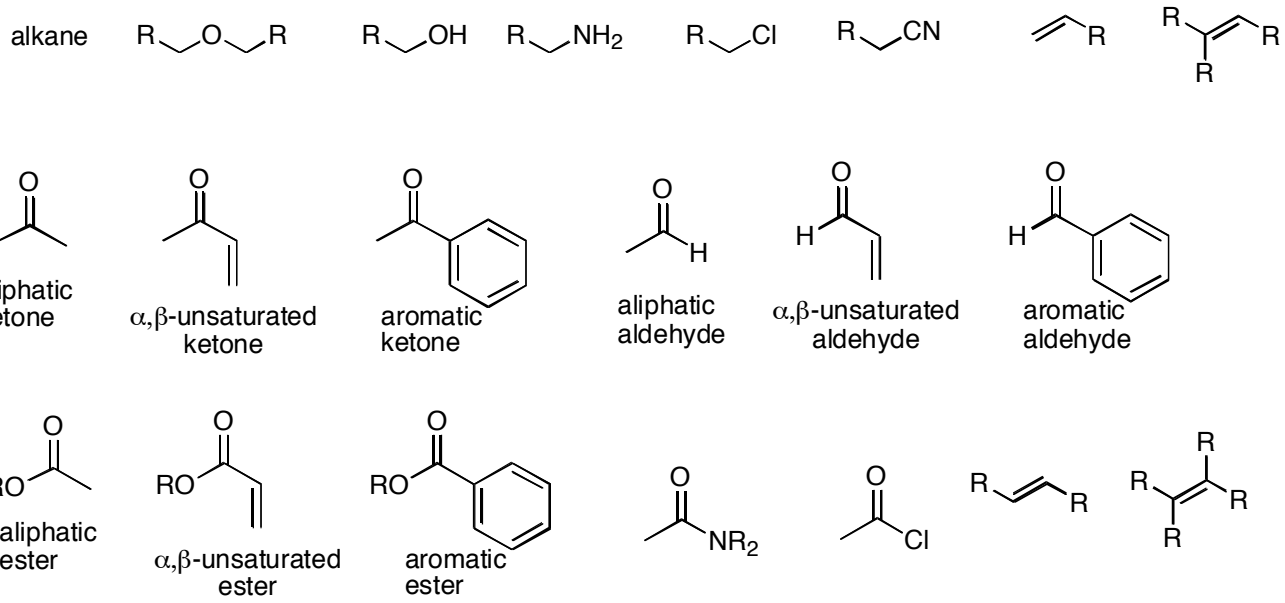
^{13}C NMR

167 (s)
163 (s)
130 (2 carbons, d)
122 (s)
114 (2 carbons, d)
73 (d)
50 (q)
39 (t)
20(q)
16.9 (t)
14 (q)

IR: 1729 cm^{-1}

a) Circle the functional group that is associated with

(i) IR: 1729 cm-1



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

7.86 ppm (d, J=8.0 Hz, 2H)
6.88 ppm (d, J=8.0 Hz, 2H)

5. Elucidate the following structure (continued)

AD: $C_{13}H_{18}O_3$

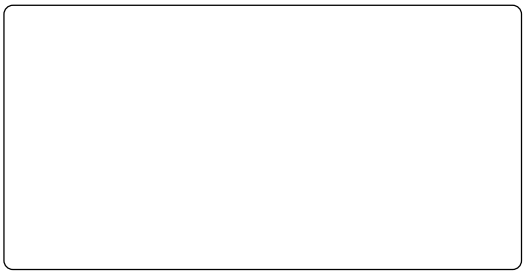
7.86 ppm (d, J=8.0 Hz, 2H)
6.88 ppm (d, J=8.0 Hz, 2H)
3.86 ppm (m, 1H)
3.91 (s, 3H)
1.67 (m, 2H)
1.43 (d, J=7.0 Hz, 3H)
1.33 (m, 2H)
0.96 (t, J=6.9 Hz, 3H)

^{13}C NMR

167 (s)
163 (s)
130 (2 carbons, d)
122 (s)
114 (2 carbons, d)
73 (d)
50 (q)
39 (t)
20(q)
16.9 (t)
14 (q)

IR: 1729 cm^{-1}

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



for answers: see Chem 334, 2008, exam 1: http://www.udel.edu/chem/fox/chem334Spring2009.html

3. Elucidate the following structure

$C_{10}H_9O_2Cl$

^{1}H NMR
7.71 (dd, *J*=7.7, 2.2 Hz, 1H)
7.44 (dd, *J*=8.1, 2.2 Hz, 1H)
6.95 (dd, *J*=8.1, 7.7 Hz, 1H)
4.81 (dd, J= 10.5, 8.9Hz, 1H)
4.20 (dd, J= 8.9, 7.3Hz, 1H)
3.60 (m, 1H)
1.34 (d, J= 9.2Hz, 3H)

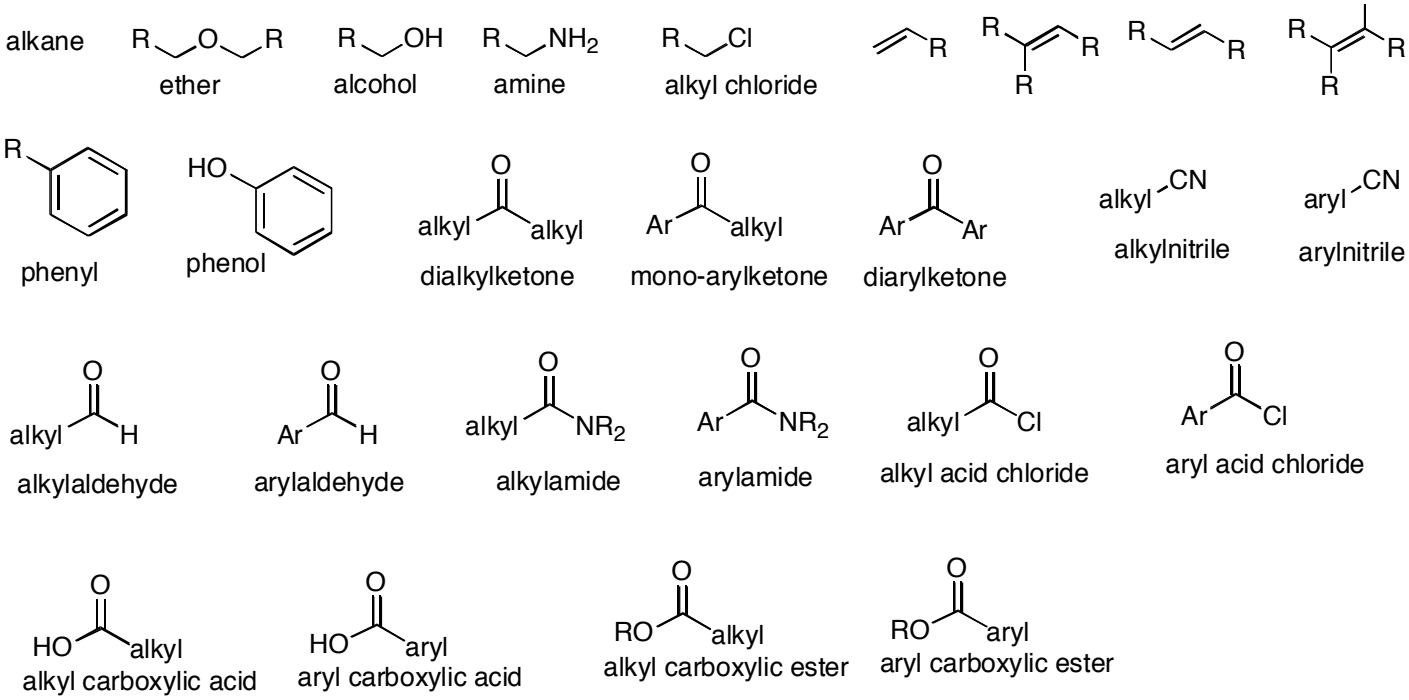
^{13}C NMR
165.7 (s)
160.6 (s)
135.4 (s)
130.2 (d)
128.9 (d)
120.5 (d)
113.5 (s)
79.5 (t)
35.9 (d)
19.2 (q)

IR: 1775 cm^{-1}

a) Circle the functional group that is associated with

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

(i) IR: 1775 cm^{-1} (8 points)



3. Elucidate the following structure (continued)

$C_{10}H_9O_2Cl$

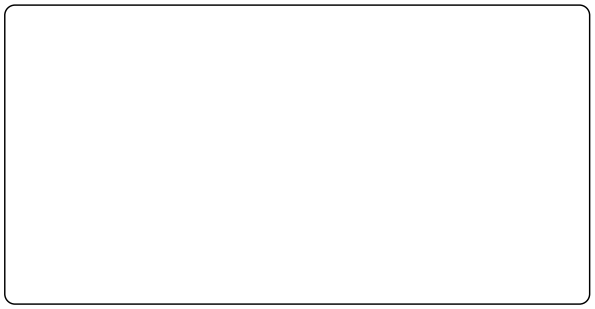
^{1}H NMR
7.71 (dd, *J*=7.7, 2.2 Hz, 1H)
7.44 (dd, *J*=8.1, 2.2 Hz, 1H)
6.95 (dd, *J*=8.1, 7.7 Hz, 1H)
4.81 (dd, J= 10.5, 8.9Hz, 1H)
4.20 (dd, J= 8.9, 7.3Hz, 1H)
3.60 (m, 1H)
1.34 (d, J= 9.2Hz, 3H)

^{13}C NMR
165.7 (s)
160.6 (s)
135.4 (s)
130.2 (d)
128.9 (d)
120.5 (d)
113.5 (s)
79.5 (t)
35.9 (d)
19.2 (q)

IR: 1775 cm^{-1}

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

(20 points)



c. Assign the following coupling constants: (15 points)

7.71 (dd, *J*=7.7, 2.2 Hz, 1H)
7.44 (dd, *J*=8.1, 2.2 Hz, 1H)
6.95 (dd, *J*=8.1, 7.7 Hz, 1H)

d. Assign the following coupling constants: (15 points)

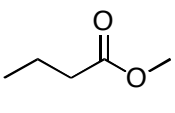
4.81 (dd, J= 10.5, 8.9Hz, 1H)
4.20 (dd, J= 8.9, 7.3Hz, 1H)
3.60 (m, 1H)
1.34 (d, J= 9.2Hz, 3H)

HINT: the peak at 3.60 is coupled to the peaks at 4.81, 4.20 and 1.34

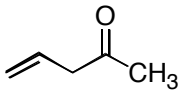
for answers: see Chem 334, 2008, exam 1: http://www.udel.edu/chem/fox/chem334Spring2009.html

2. Match the following ^{13}C NMR spectra with one of the following substances. Write you answer in the box along side the spectrum Multiplicities [I.e. (s,d,t,q)] are indicated above each peak.

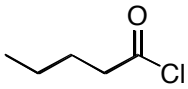
(18 points)



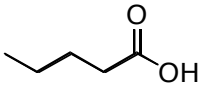
A



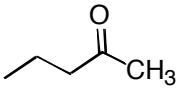
B



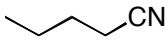
C



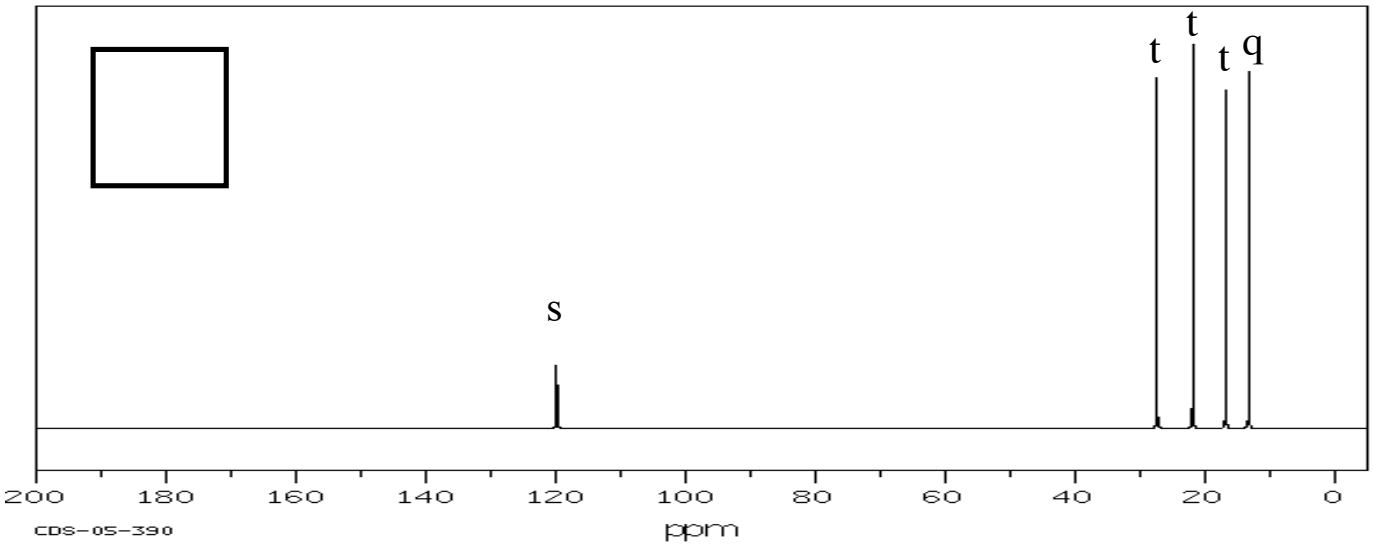
D

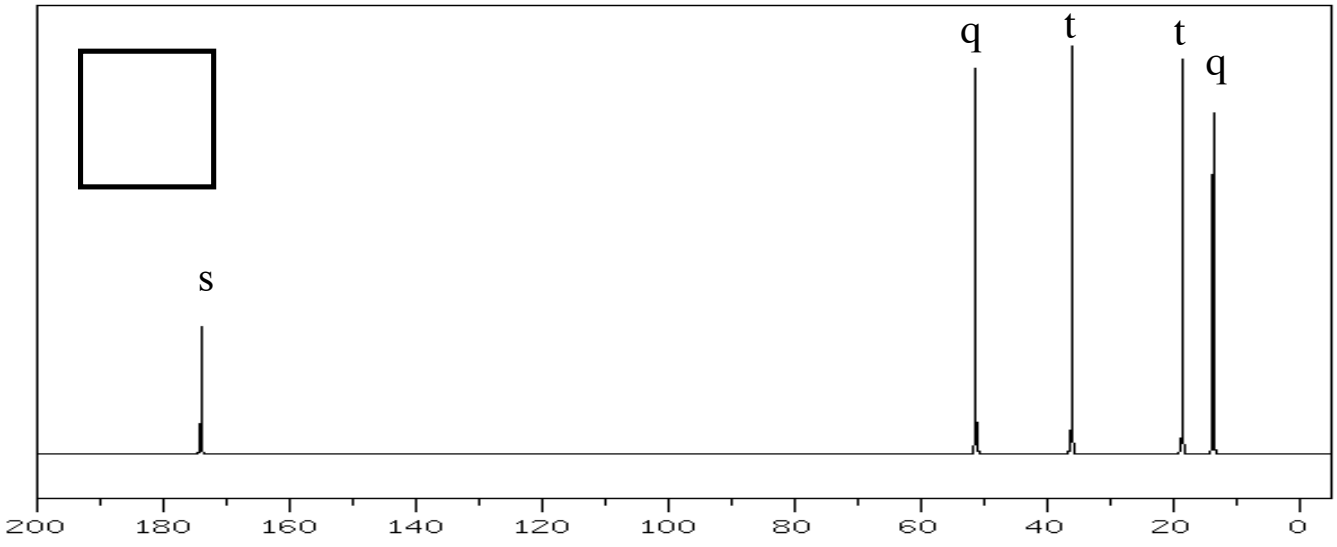


E



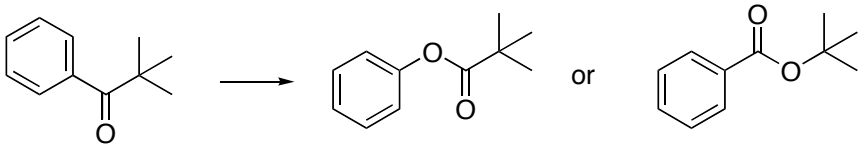
F





for answers: see Chem 334, 2009, exam 1: http://www.udel.edu/chem/fox/chem334Spring2009.html

3. Oxidation of **D** could lead to either **E** or **F.** Explain how you would use ^{13}C NMR to distinguish these compounds. (12 points)

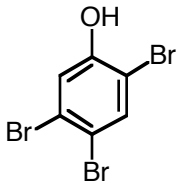


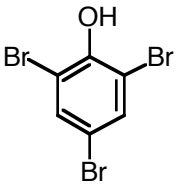
D **E** **F**

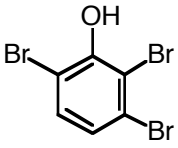
for answers: see Chem 334, 2008, exam 2: http://www.udel.edu/chem/fox/chem334Spring2009.html

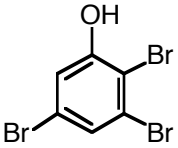
Name_____

1. Match each structure with the correct spectrum





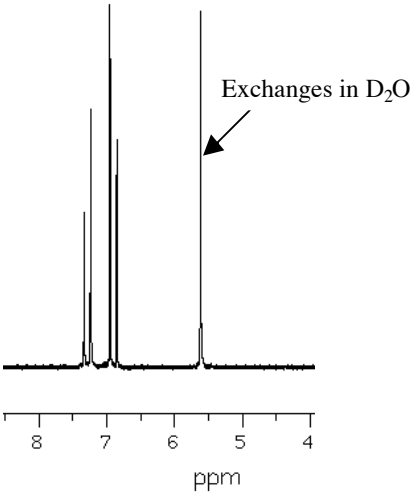




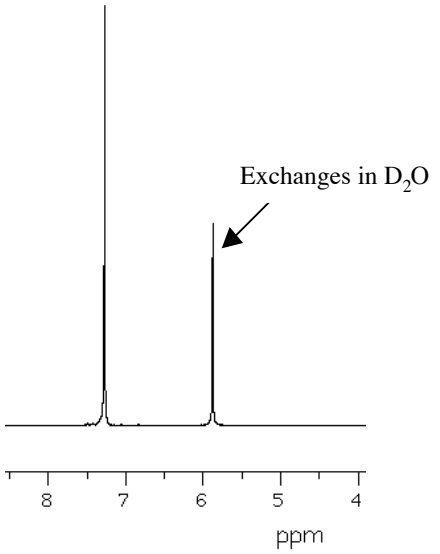
_____ _____ _____ _____

write the answers on these lines

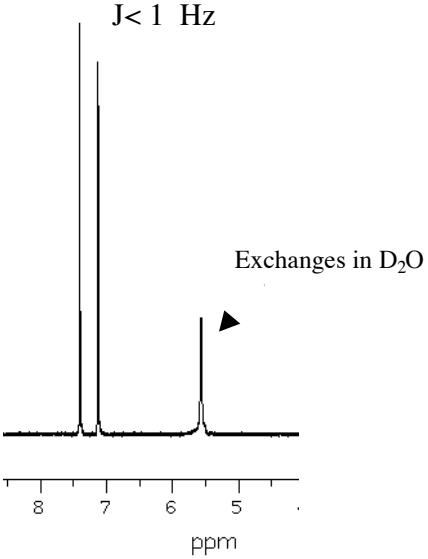
a *J*= 9.0 Hz



b



c J< 1 Hz



d J= 2.4 Hz