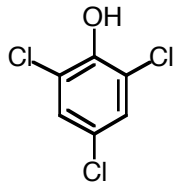
Chem 333
Final Exam
Dec 14, 2001
Professor Fox

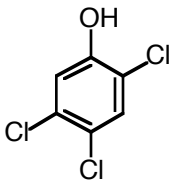
Write your name on every page
200 points

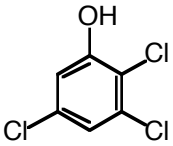
Name_____

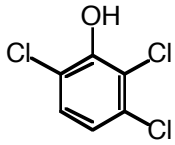
Name_____

1. (16 points) Match each structure with the correct spectrum





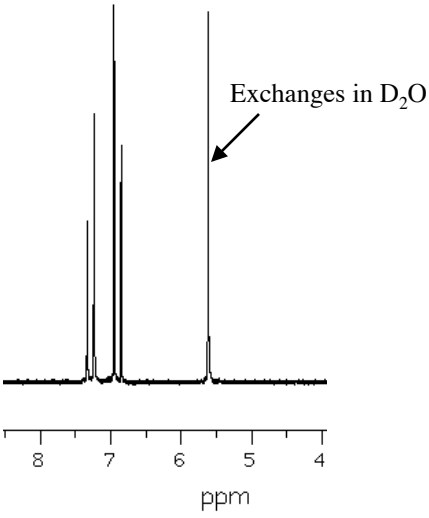




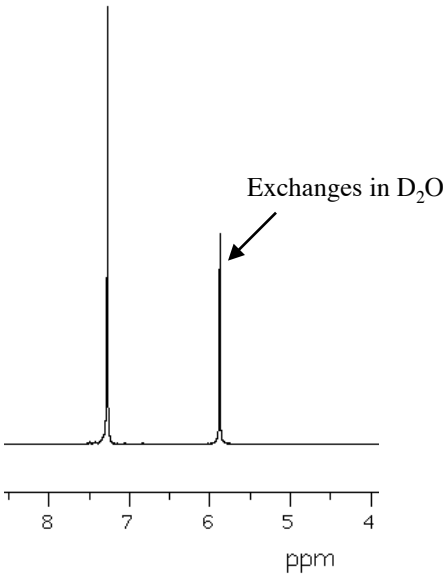
_____ _____ _____ _____

write the answers on these lines

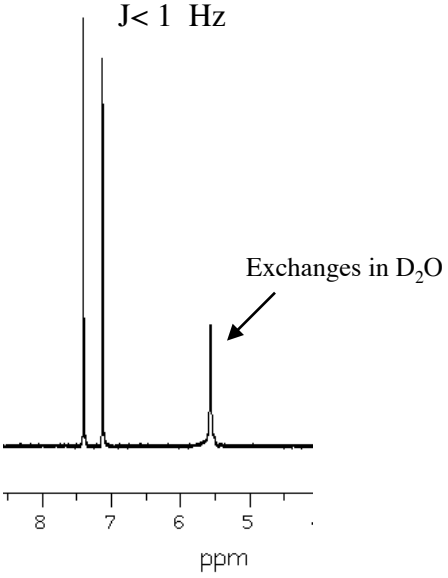
a *J*= 9.0 Hz



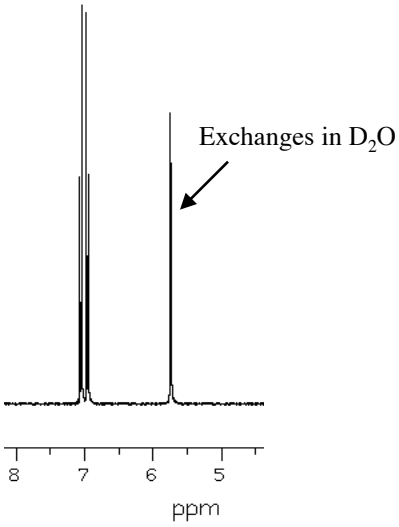
b



c J< 1 Hz

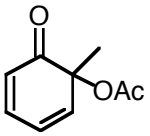


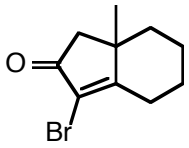
d J= 2.4 Hz

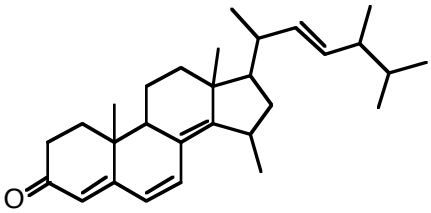


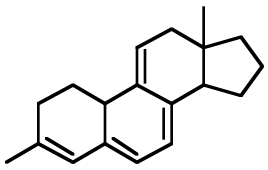
Name_____

2. Calculate the UV maximum for the following compounds. (20 points)



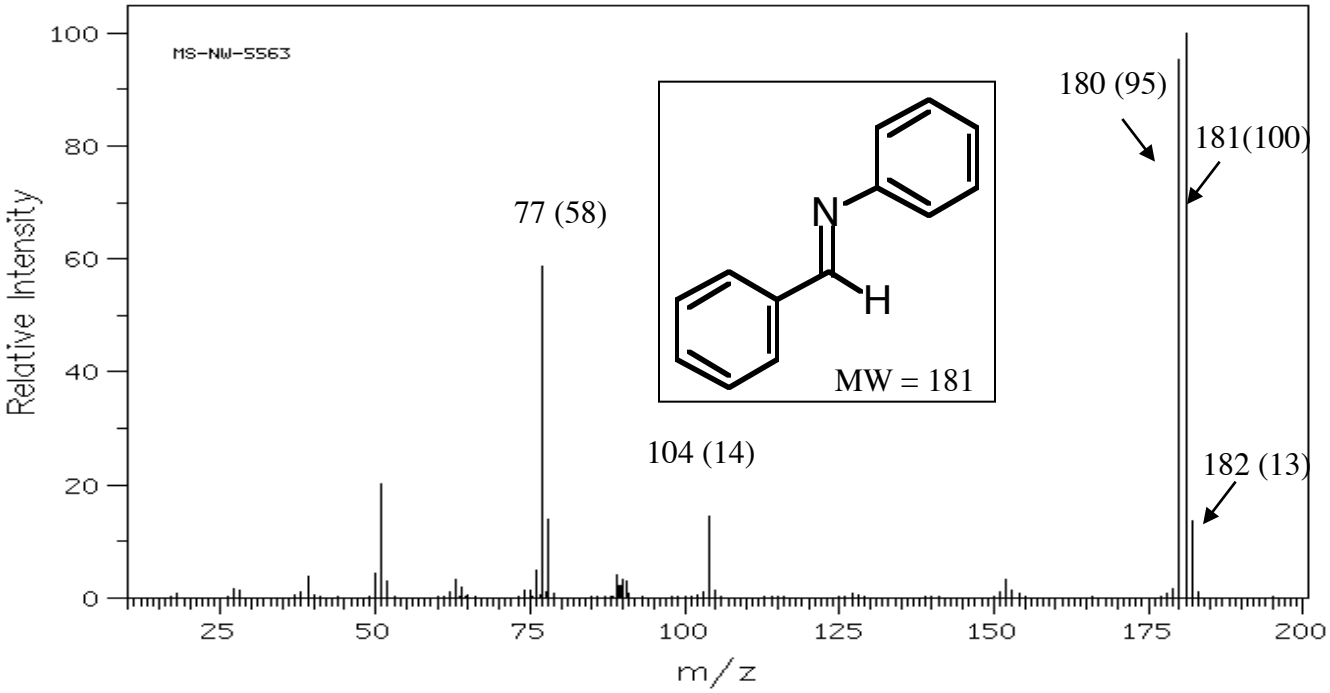






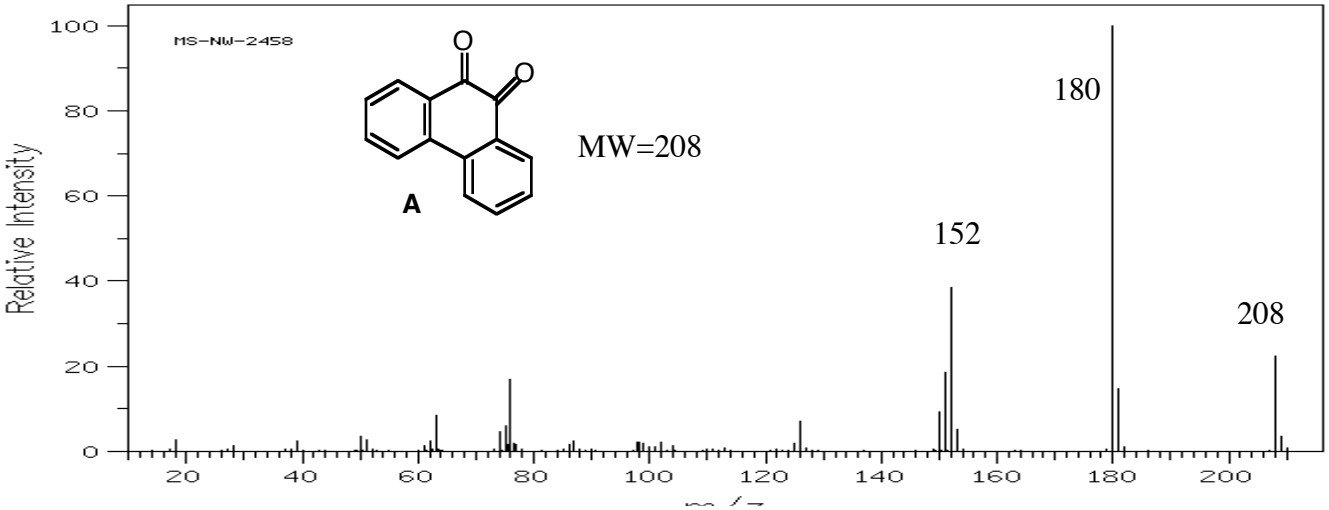
Name_____

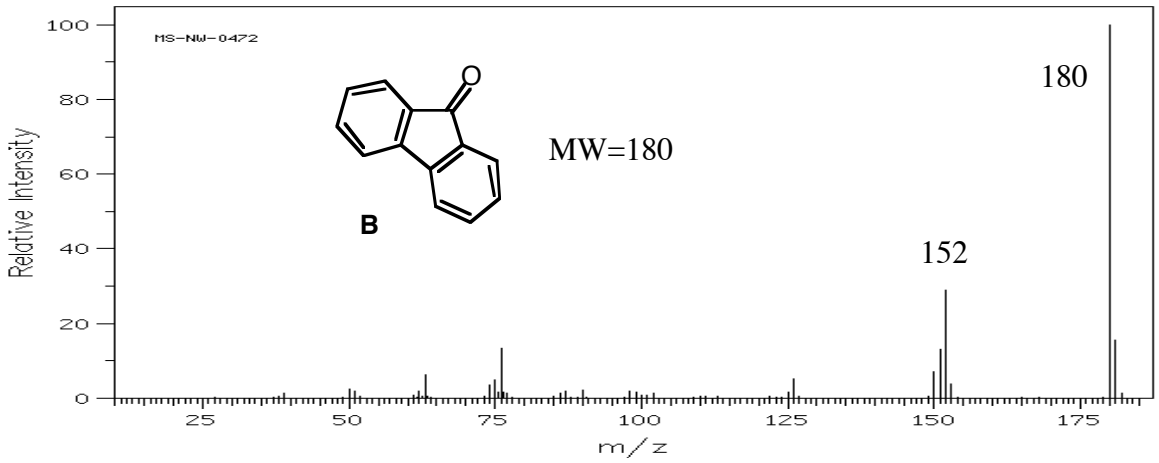
3. Explain how the labeled fragments are formed. Relative intensities are given in parentheses. (20 points)



Name_____

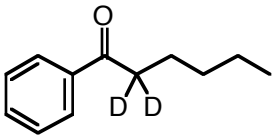
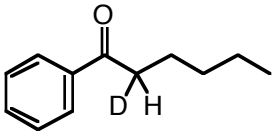
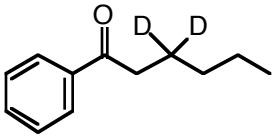
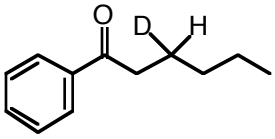
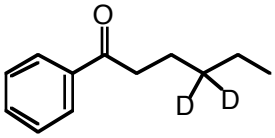
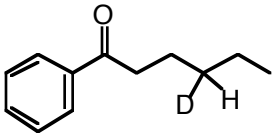
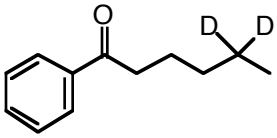
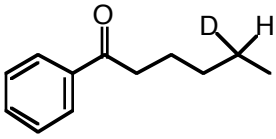
4. The mass spectra of compounds **A** and **B** are nearly identical, except for the additional peak at 208 in the spectrum of **A**. Explain why, and in doing so assign the labeled peaks in the mass spectrum. (20 points)





Name_____

5. McLafferty rearrangements of the molecules depicted below will give rise to fragments that can be detected by mass spectrometry. Circle the fragments that are observed. You may need to circle more than one answer for each! (24 points)

	120	121	122
	120	121	122
	120	121	122
	120	121	122
	120	121	122
	120	121	122
	120	121	122
	120	121	122

READ CAREFULLY!

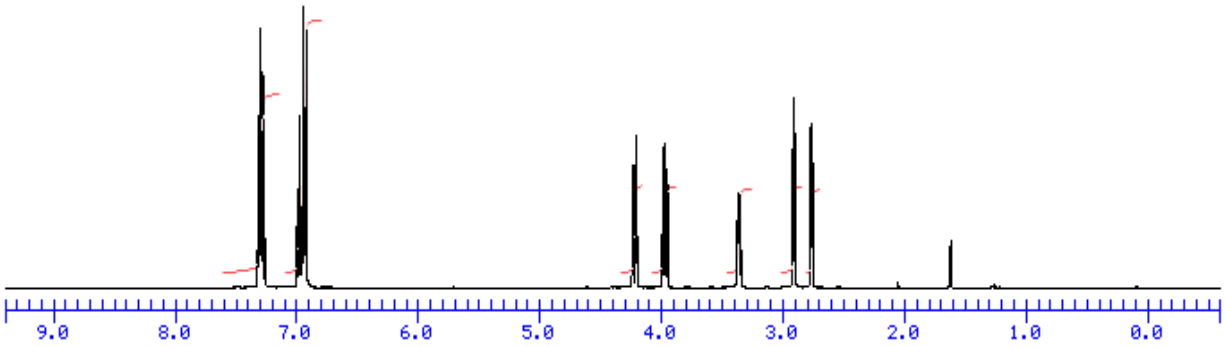
To receive full credit for question 6, clearly show your rationale for elucidating the structure. In addition, all ^{1}H and ^{13}C NMR chemical shifts, as well as ^{1}H coupling constants must be assigned and displayed in the designated blocks. This will involve drawing your final structure at least 3 times. Simply drawing the structure of the product will get you no credit.

To receive full credit for question 7, clearly show your rationale for elucidating the structure. In addition, all ^{1}H and ^{13}C NMR chemical shifts, as well as ^{1}H coupling constants must be assigned and displayed in the designated blocks. This will involve drawing your final structure at least 3 times. Furthermore, assign at least **2** peaks associated with the **main** functional groups in the IR spectrum. Also, assign the bolded numbers in the mass spectrum. Simply drawing the structure of the product will get you no credit.

Name_____

6. $C_9H_{10}O_2$ (50 points)

^{1}H NMR	^{13}C NMR
7.30, m, 2H	158.5, s
6.95, m, 3H	129.5, d (2)
4.22, dd, 1H, J=3.5, 11.3 Hz	121.3, d
3.97, dd, 1H, J=5.7, 11.3 Hz	114.7, d,(2)
3.36, m, 1H	68.7, t
2.91, dd, 1H, J=4.4, 5.2 Hz	50.2, d
2.76, dd, 1H, J=3.3, 5.2 Hz	44.7, t



Question 6 continued

Name_____

Name_____

Question 6 continued

^{13}C chemical shift assignments

^{1}H Chemical shift assignments

^{1}H coupling constant assignments

Name_____

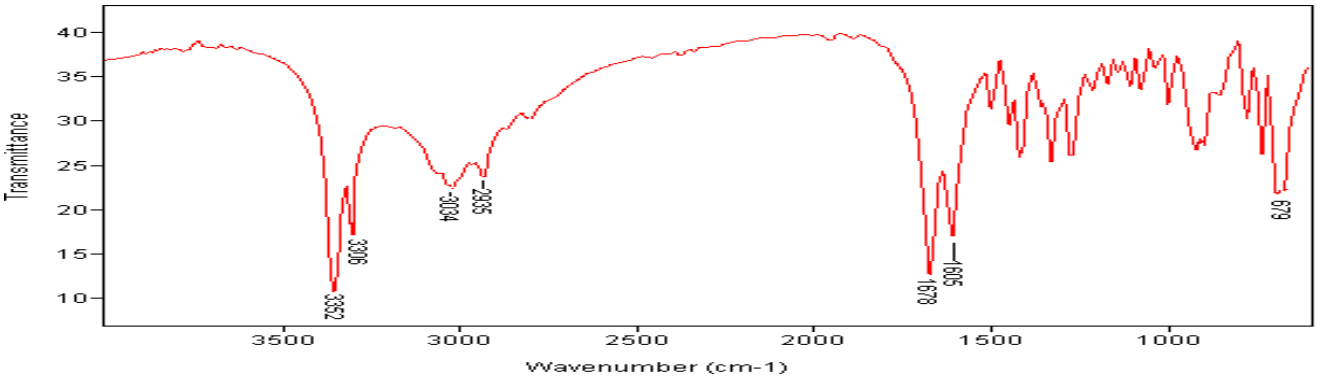
7. $C_9H_{12}N_2O$ (50 points)

^{1}H NMR
6.86. bs, 1H
6.83-6.72, m, 5H
6.5. bs. 1H
2.88, dd, 1H, J=5.7, 8.6 Hz
2.45, dd, 1H, J= 5.7, 13.3 Hz
2.14, dd, 1H, J=8.6, 13.3 Hz
1.1, bs, 2H

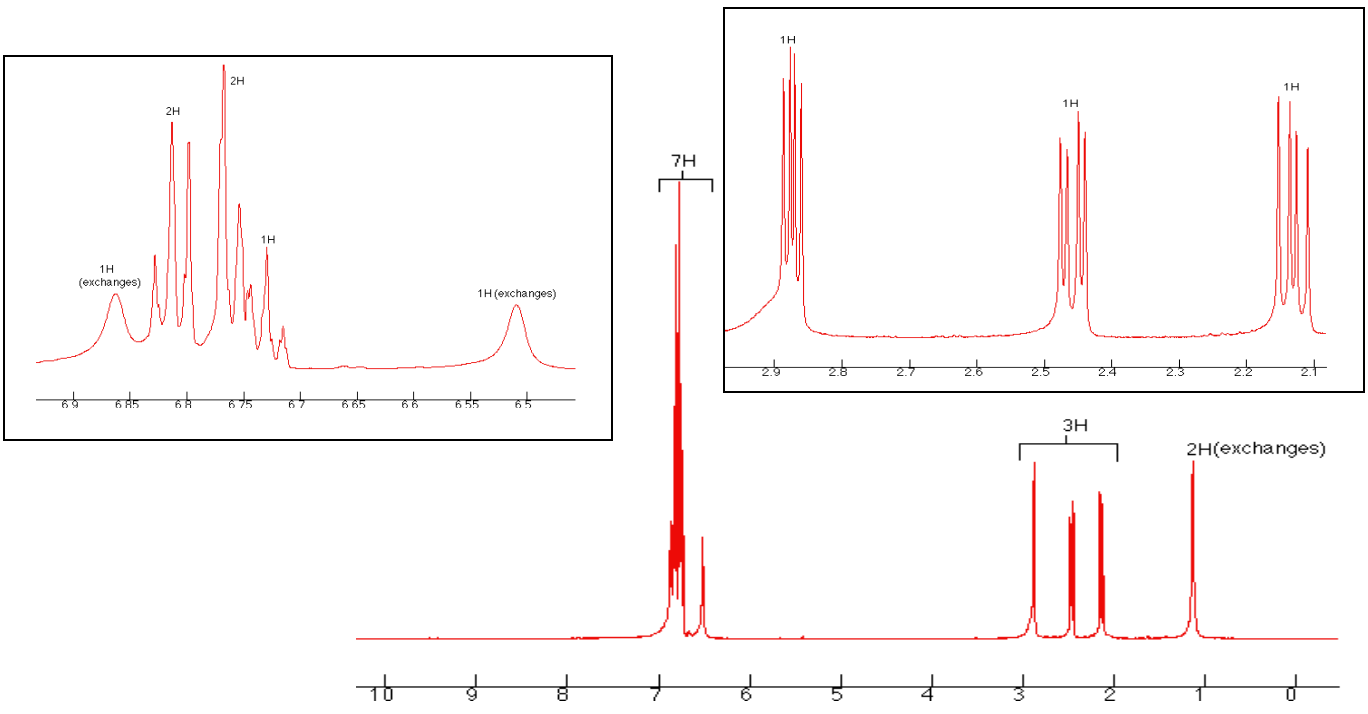
^{13}C NMR
176.7, s
138.9, s
129.3, d (2)
128.0, d (2)
126.0, d
56.2, d
41.2, t

MS:
164(15), 147(4),
146(4), **120**(100),
103(12), **91**(13),
73(19), 65(5),
51(2), 28(4), 18(6)

IR



^{1}H NMR (500 MHz)



Question 7 continued Name_____

^{13}C chemical shift assignments

^{1}H Chemical shift assignments

^{1}H coupling constant assignments

IR assignments

Question 7 continued

Name_____

Mass Spec assignments