

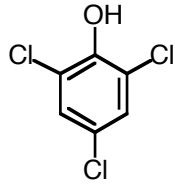
Chem 333
Final Exam
Dec 14, 2001
Professor Fox

Write your name on every page
200 points

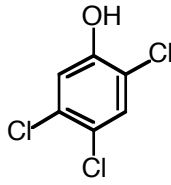
Name _____

Name _____

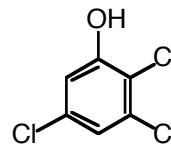
1. (16 points) Match each structure with the correct spectrum



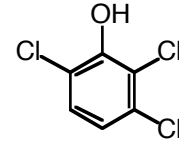
b



c

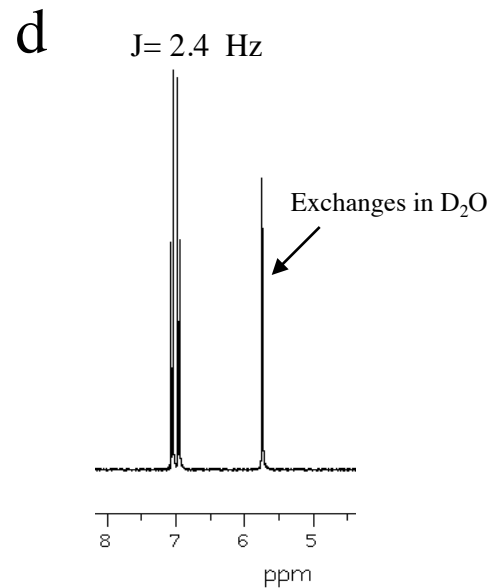
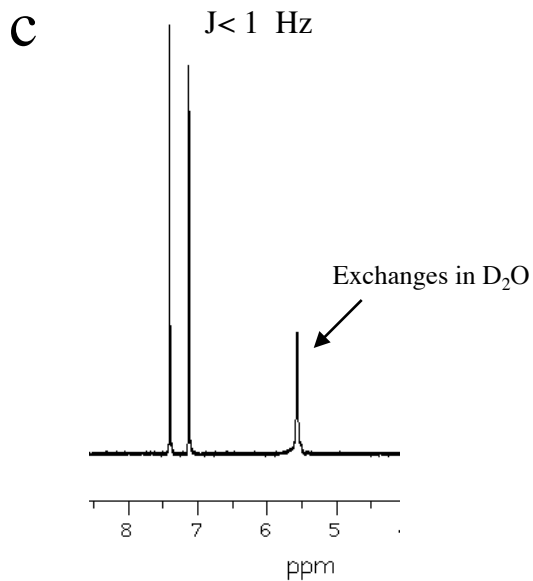
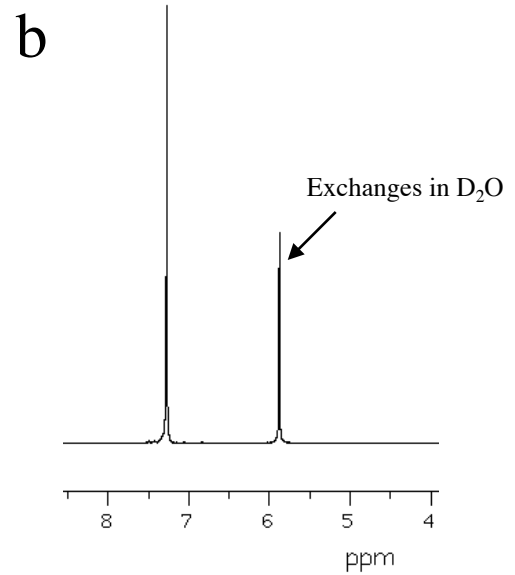
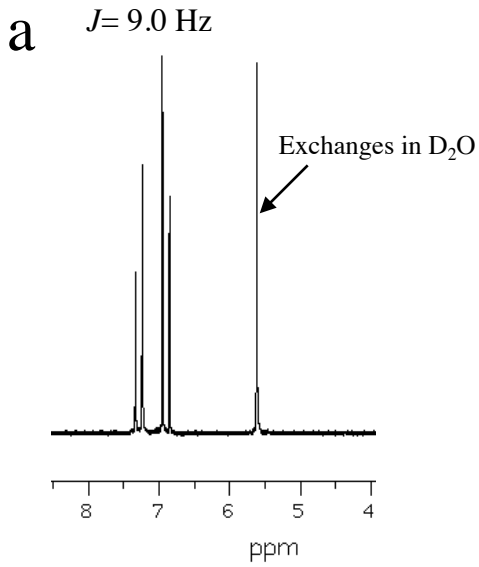


d



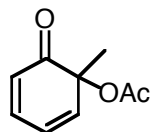
a

write the answers
on these lines

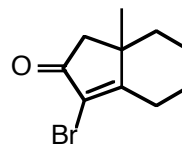


Name _____

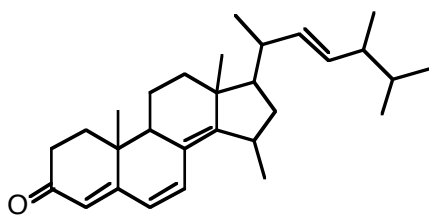
2. Calculate the UV maximum for the following compounds. (20 points)



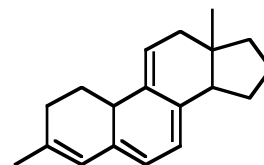
Base	215
Double bond extension(DBE)	30
δ alkyl	18
homodiene	39
<hr/>	
	302 nm



Base	202
α bromo	25
2 β alkyls	24
Exocyclic olefin	5
<hr/>	
	256 nm



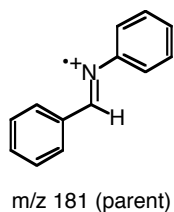
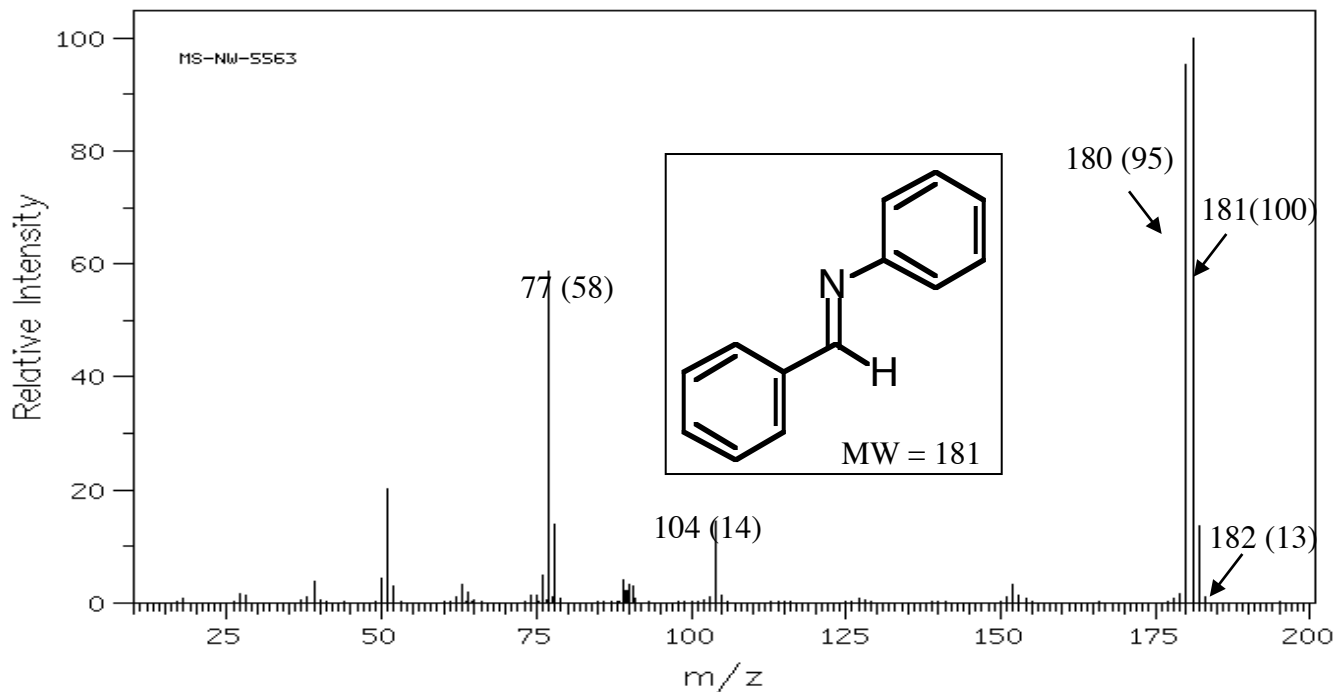
Base	215
2 DBE	60
β alkyl	54
3 $>\gamma$ alkyl	39
3 exocyclic olefins	15
<hr/>	
	356 nm



Base(homodiene)	253
2 DBE	60
6 alkyls	30
3 exocyclic olefins	15
<hr/>	
	358 nm

Name _____

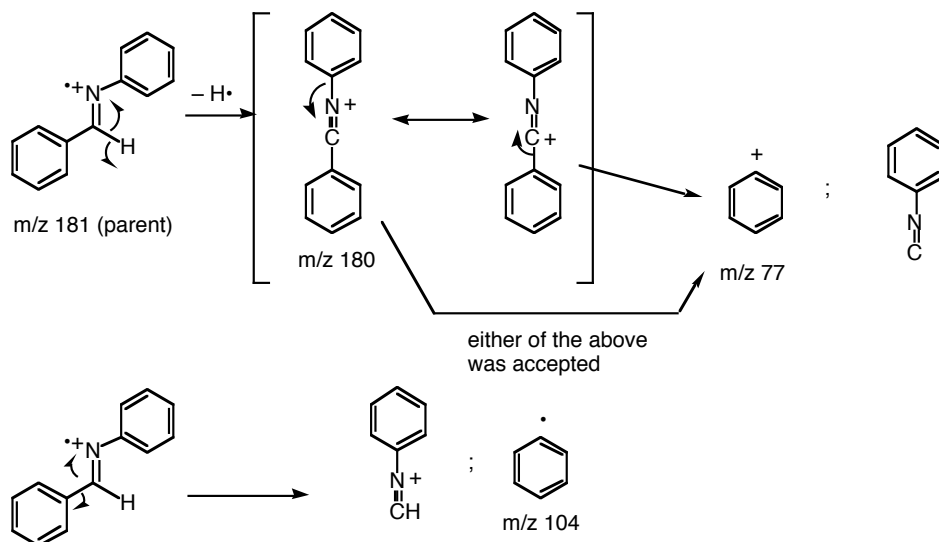
3. Explain how the labeled fragments are formed. Relative intensities are given in parentheses. (20 points)



$(C^{12})_{12}(C^{13})_1H_{11}N$

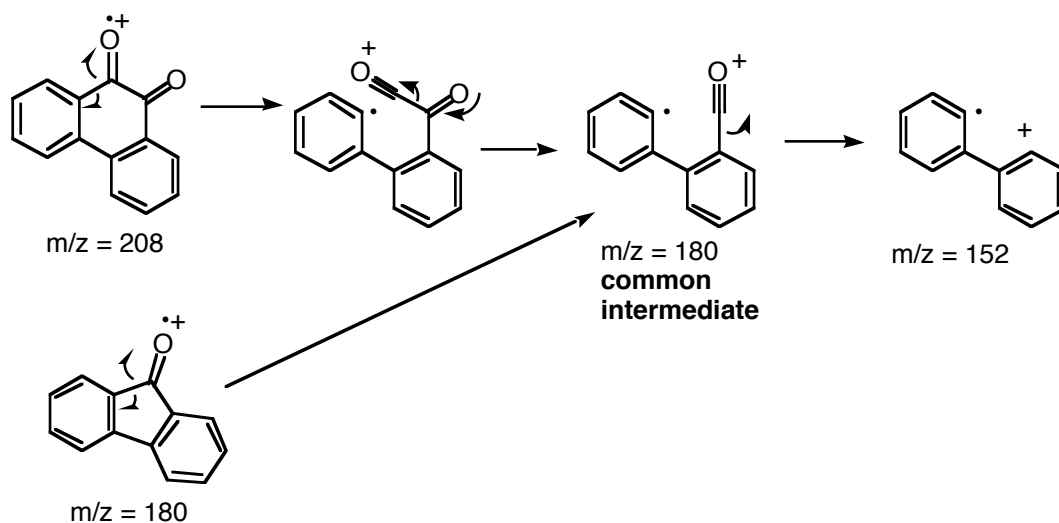
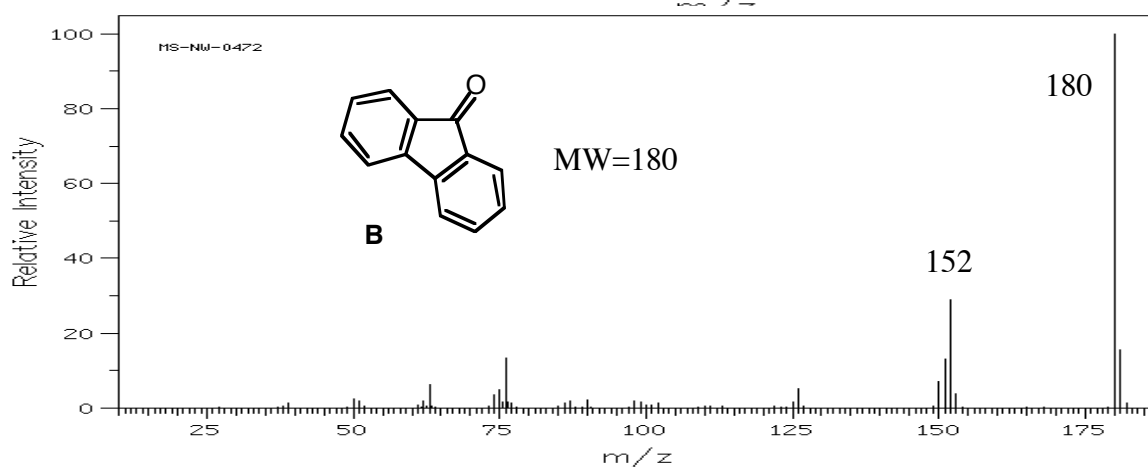
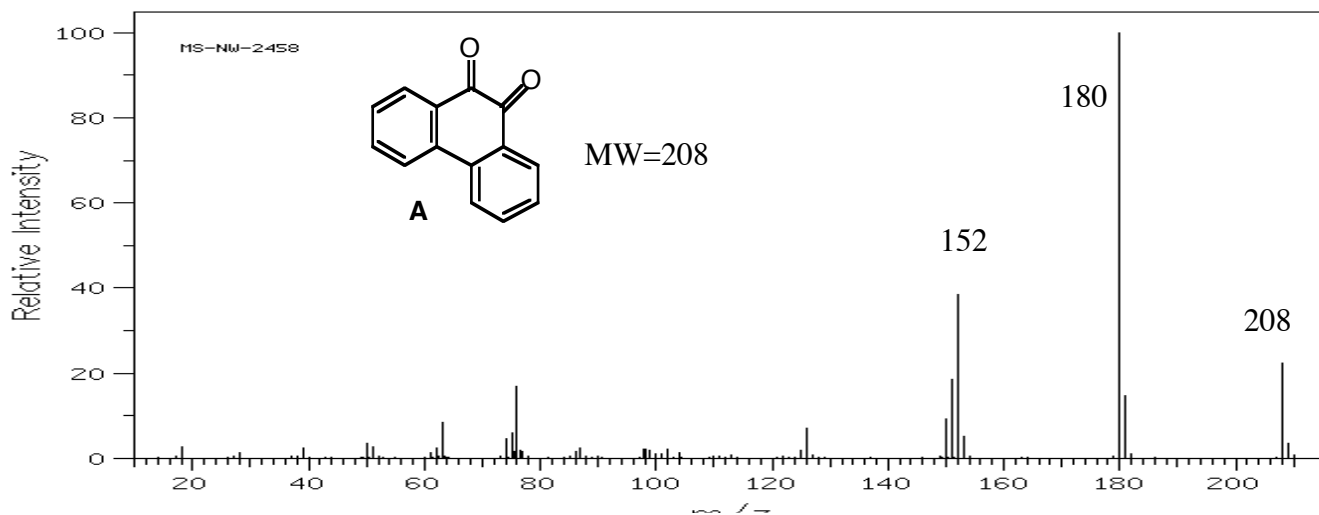
m/z 182

ratio of the parent peak to this peak
is 100:13, because there are 13 carbons
in the molecule, and the natural abundance
of C^{13} is ca. 1%.



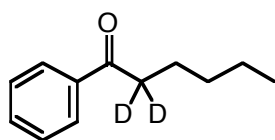
Name _____

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 _____

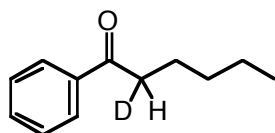
5. McLafferty rearrangements of the molecules depicted below will give rise to fragments that can be detected by mass spectrometry. Circle the fragments that are observed. You may need to circle more than one answer for each! (24 points)



120

121

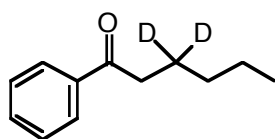
122



120

121

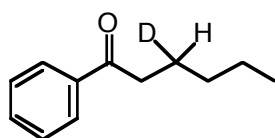
122



120

121

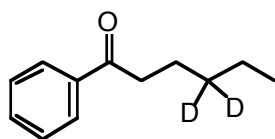
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120

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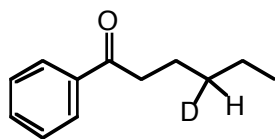
122



120

121

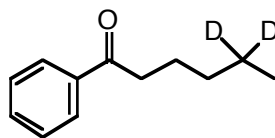
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120

121

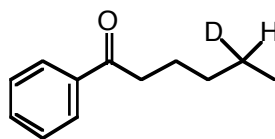
122



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 ^1H and ^{13}C NMR chemical shifts, as well as ^1H 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 ^1H and ^{13}C NMR chemical shifts, as well as ^1H 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)

1H NMR

7.30, m, 2H

6.95, m, 3H

4.22, dd, 1H, $J=3.5, 11.3$ Hz

3.97, dd, 1H, $J=5.7, 11.3$ Hz

3.36, m, 1H

2.91, dd, 1H, $J=4.4, 5.2$ Hz

2.76, dd, 1H, $J=3.3, 5.2$ Hz

^{13}C NMR

158.5, s

129.5, d (2)

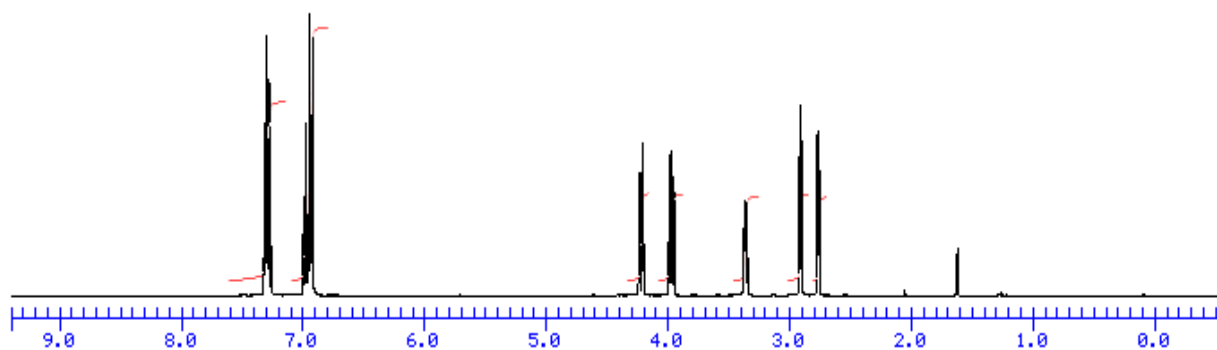
121.3, d

114.7, d,(2)

68.7, t

50.2, d

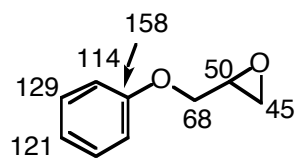
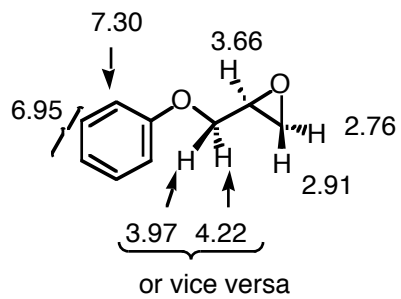
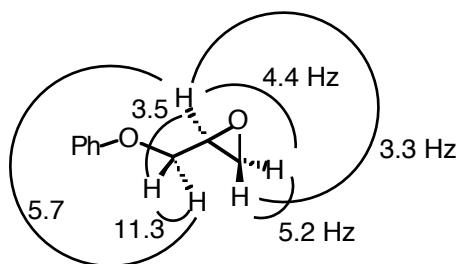
44.7, t



Question 6 continued

Name _____

Question 6 continued

¹³C chemical shift assignments¹H Chemical shift assignments¹H coupling constant assignments

7. C₉H₁₂N₂O (50 points)

Name _____

¹H 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

¹³C 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),

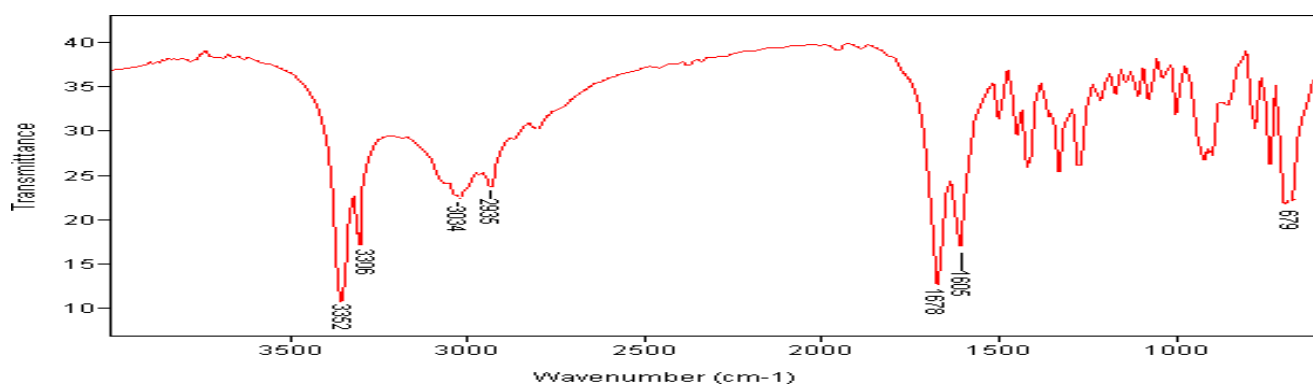
146(4), **120**(100),

103(12), **91**(13),

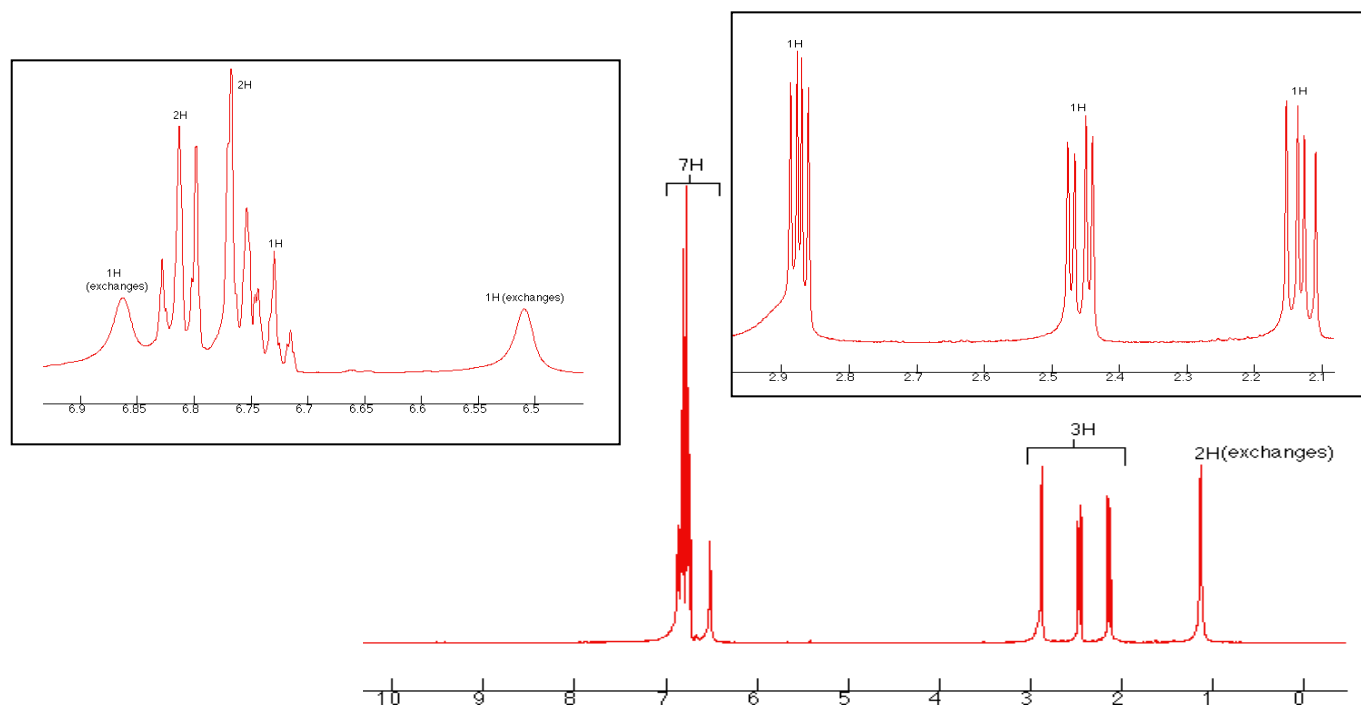
73(19), 65(5),

51(2), 28(4), 18(6)

IR

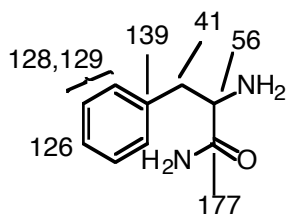
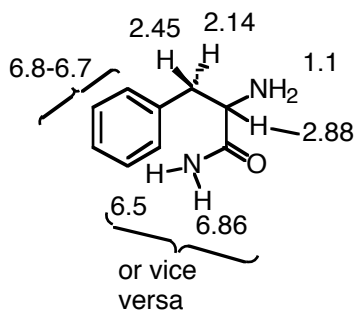
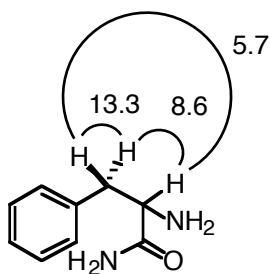


¹H NMR (500 MHz)



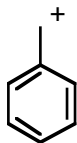
Question 7 continued

Name _____

¹³C chemical shift assignments¹H Chemical shift assignments¹H coupling constant assignments

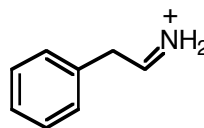
IR assignments

Various accepted

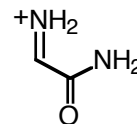


m/z = 91
need to have a
terminal phenyl group

MS assignments

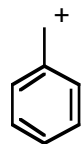


m/z = 120

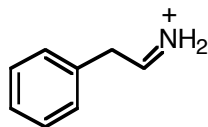


m/z = 73

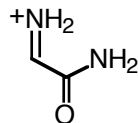
Mass Spec assignments



$m/z = 91$
need to have a
terminal phenyl group



$m/z = 120$



$m/z = 73$