Chem 331, Fall 08

William Jenks

Name_____

PLEASE ALSO WRITE YOUR NAME ON THE TOP OF THE BACK OF YOUR EXAM

Please check off which recitation section you attend:

_____ Friday, 9:00 a.m. (10)

_____ Friday, 11:00 a.m. (11)

_____ Monday, 11:00 a.m. (12)

_____ Monday, 2:10 p.m. (13)

_____ Tuesday, 10 a.m. (14)

MIDTERM 5
4 Dec, 2008

Problem (max score)	Score
I (27)	
II (16)	
III (17)	
IV (20)	
V (20)	
Total (100)	

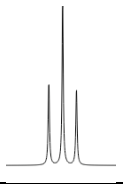
I. 27 points. Suppose you take a mass spectrum of a sample that results in a molecular ion M^+ of mass 142.

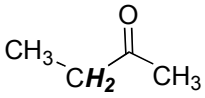
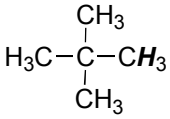
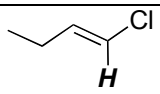
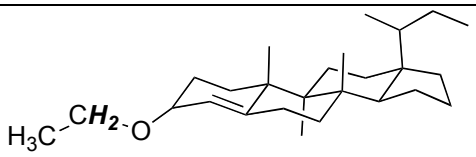
(a) Draw three molecules <u>each with a different molecular formula</u> that correspond to this mass, one in each of the three top boxes

(b) Fill in the rest of the boxes, according to your answers for part (a).

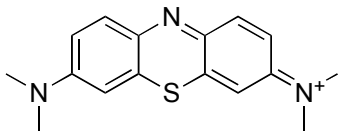
Molecule A	Molecule B	Molcule C
How many unsaturations in A?	How many unsaturations in B?	How many unsaturations in C?
Is A chiral?	Is B chiral?	Is C chiral?
How many ^{13}C signals for A?	How many ^{13}C signals for B?	How many ^{13}C signals for C?

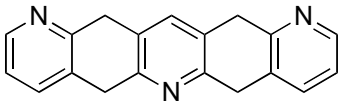
II. 16 points. Sketch the expected appearance of the signal that corresponds to the hydrogens indicated in ***boid italics***. A sample answer might look like the illustration in the upper right corner of this page. Quality of art DOES count!

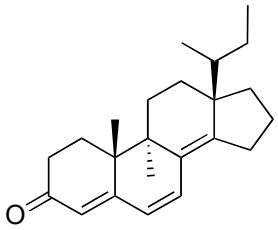


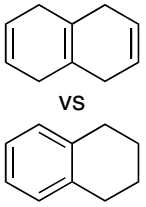
III. 5 points. Circle the molecule from the choices below that absorbs visible light.





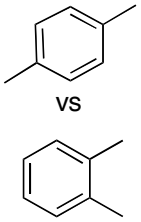


12 points. For each of the pairs of molecules below, indicate whether each of the given spectroscopic methods would *easily* discriminate between the compounds, i.e., if you had the spectrum in front of you and knew that the real compound was one of these two compounds, could you easily tell which is was. *Circle the methods for which the answer is yes and cross out the methods for which the answer is no.*



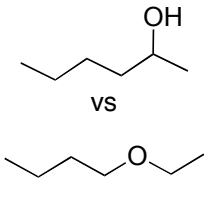
UV IR

^{1}H NMR ^{13}NMR



UV IR

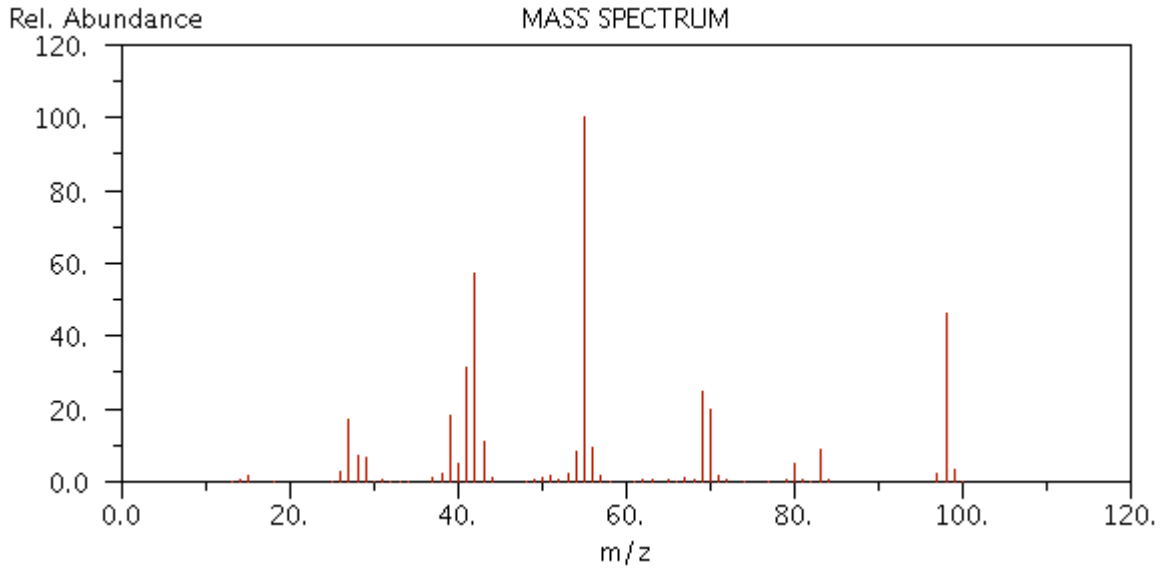
^{1}H NMR ^{13}NMR

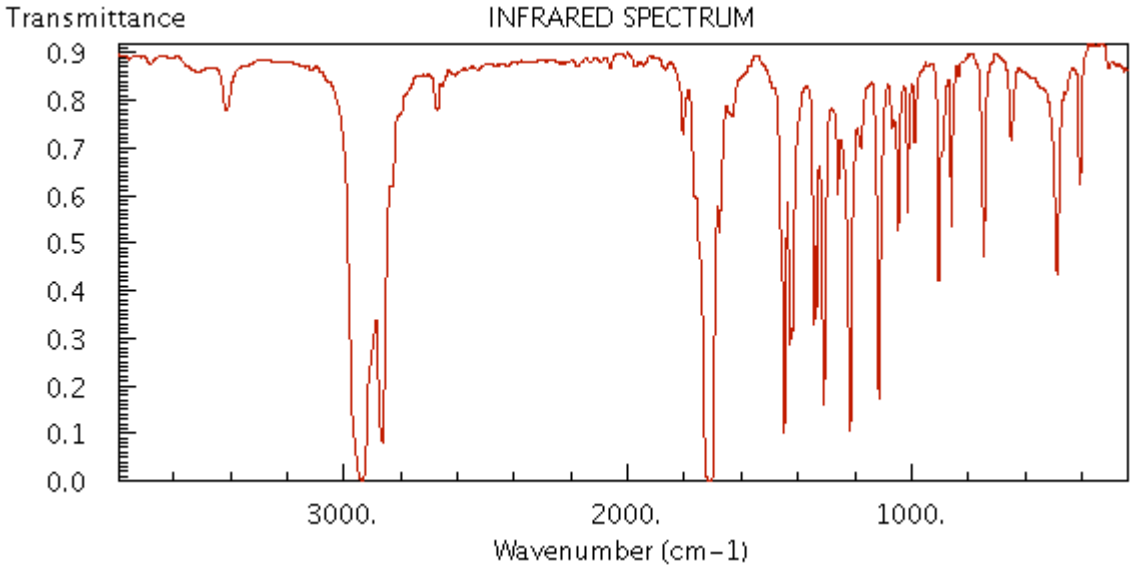


UV IR

^{1}H NMR ^{13}NMR

III 20 points. Consider the following spectra. *The molecular ion is visible on the mass spectrum*. The ^{13}C spectrum (not shown) has 4 peaks.





(a) Put a rectangular box around the molecular ion peak in the mass spectrum. Draw an arrow pointing to the base peak.

(b) Draw a reasonable structure for this molecule.

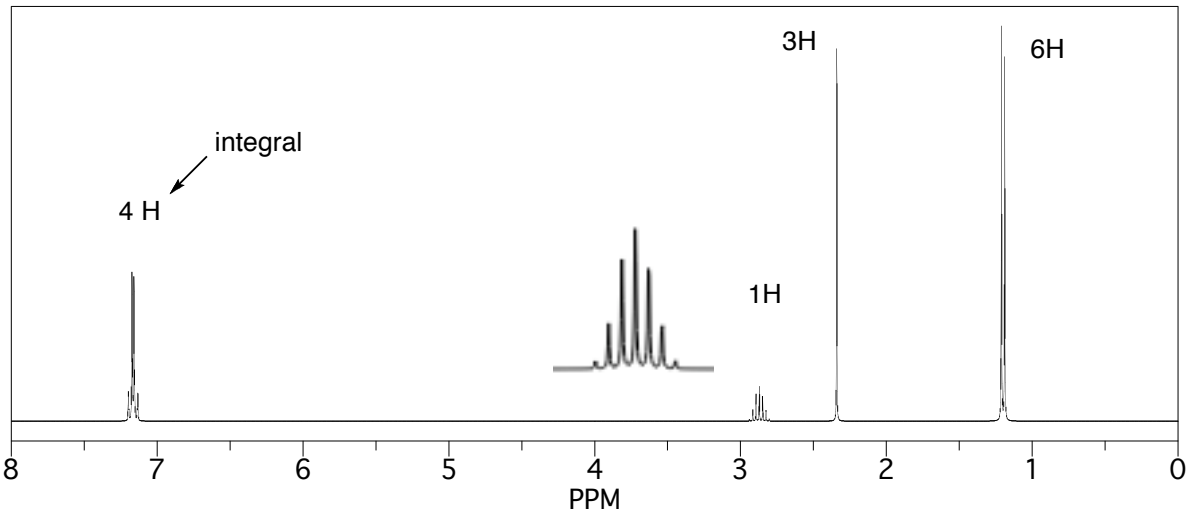
III. 20 points. The ^{1}H spectrum, IR spectrum, and ^{13}C spectrum of a hydrocarbon are shown below.

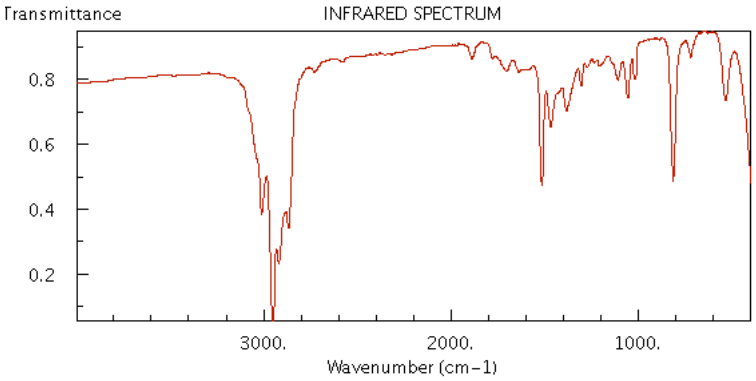
(a) Put a star next to all the peaks that indicate the presence of pi bonds in the molecule

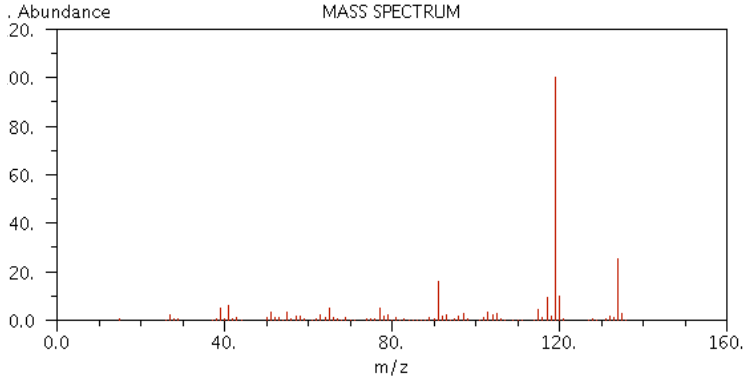
(b) The molecular weight of the compound is 134. Write down the molecular formula in the box.

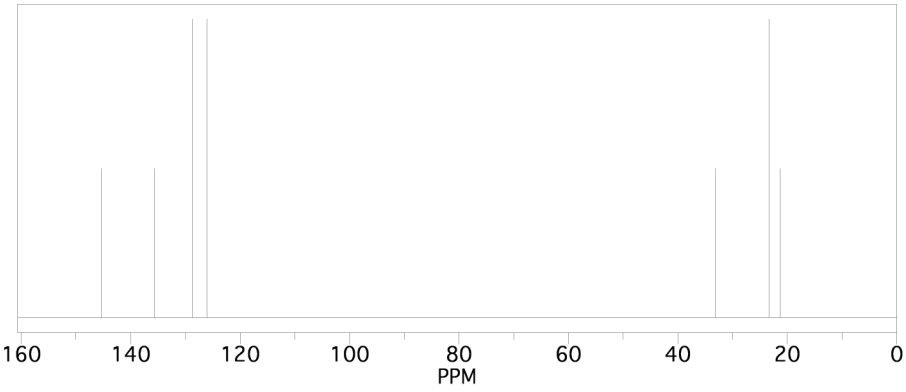
(c) What molecular fragment has been lost to give the base peak in the MS? Write down the formula of the lost fragment on the MS and circle it.

(d) Draw a reasonable molecular structure for this compound, given all of the data near the bottom of the page and circle it.



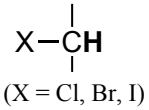
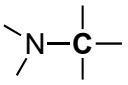
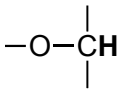
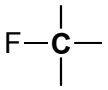
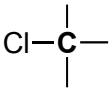
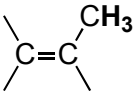
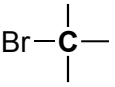
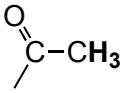
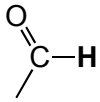
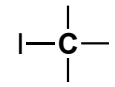
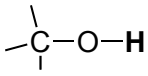
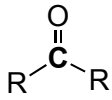
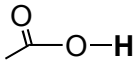
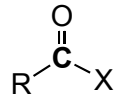
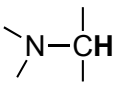
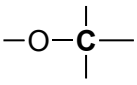






IR absorptions

Class	Group	Wavenumber (cm^{-1})
Alkane	C–H	2850-1960
Alkene	C–H	3020-3100
	C=C	1640-1680
Alkyne	C–H	3300-3320
	C≡C	2100-2260
Alcohol	O–H	3400-3650
	C–O	1050-1200
Ether	C–O	1070-1150
Aldehyde	C=O	1670-1780 "norm" ~1735
Ketone	C=O	1660-1780 "norm" ~ 1715

Partial Structure	^{1}H NMR δ (ppm)	Partial Structure	^{1}H NMR δ (ppm)	Partial Structure	^{13}C NMR δ (ppm)	Partial Structure	^{13}C NMR δ (ppm)
	0.7–1.3	 (X = Cl, Br, I)	2.5–4.0		0–30		40–60
	1.2–1.6		3.3–4.5		15–55		70–80
	1.4–1.8		4.5–6.5		25–55		25–50
	1.6–2.2	Ar-**H**	6.5–8.0		30–40		10–40
	2.0–2.4		9.7–10.0		80–145		–20–10
Ar-C**H**$_3$	2.4–2.7		2.5–5.0 (variable)	—C≡C—	70–90		190–220
—C≡C**H**	2.5–3.0		11.0–12.0	**Aromatic Carbons**	110–170	 (X= OR' or NR'$_2$)	150–180
	2.0–3.0				50–90		