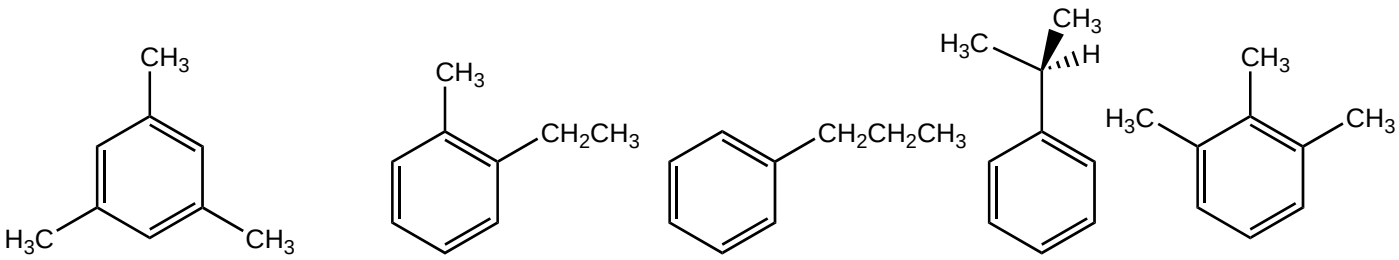
CEM 252
Summer 2006

Quiz 2 - 18 July 2006
20 points

Name_____

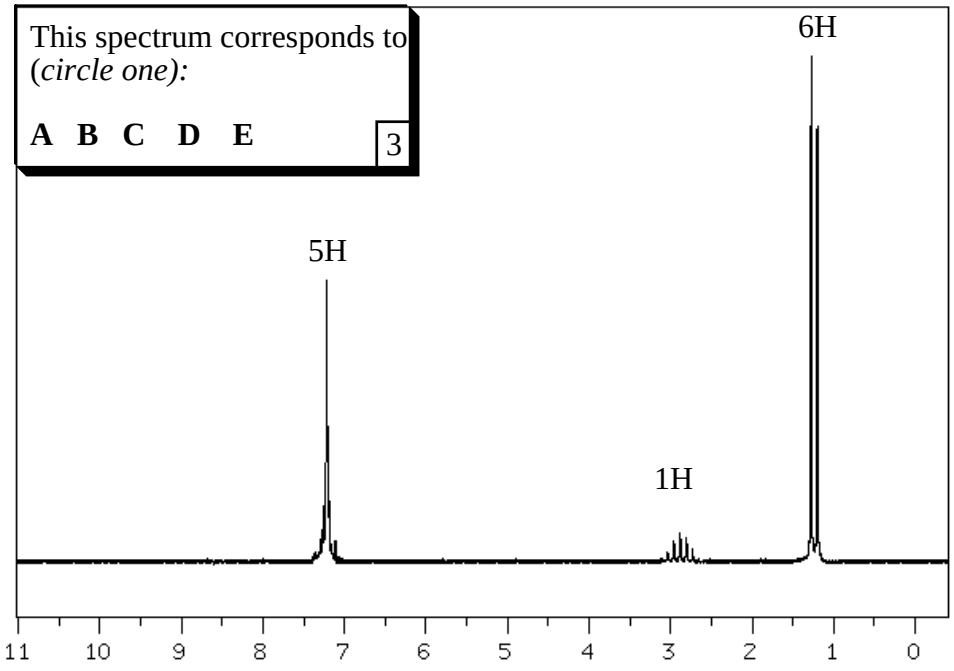
1. Match the following ^{1}H-NMR spectra to the appropriate C_9H_{12} molecule below:



A **B** **C** **D** **E**

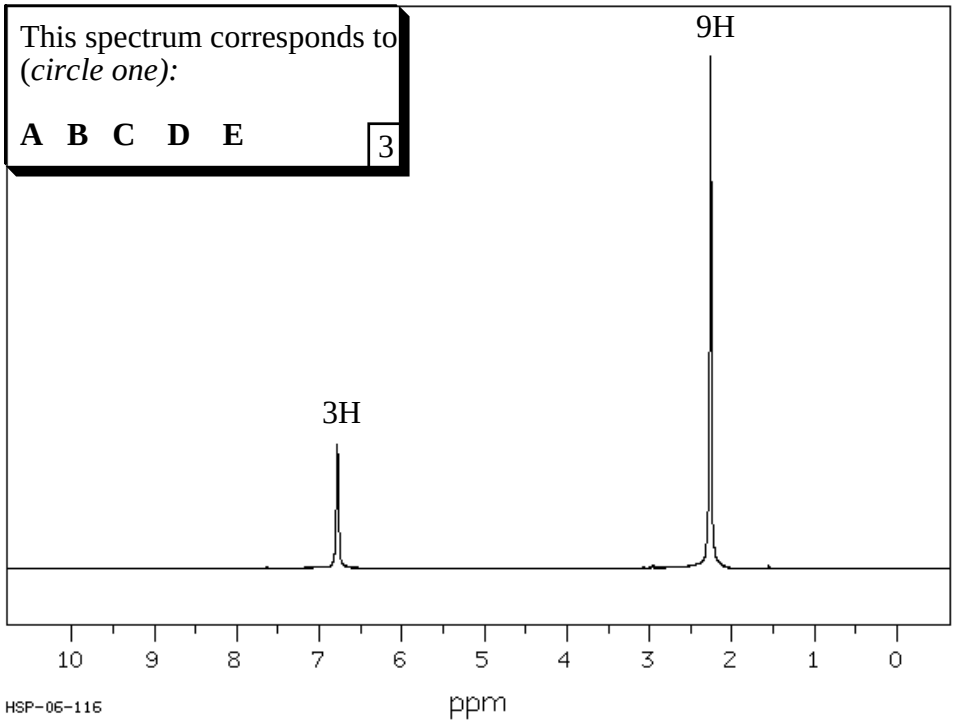
i) This spectrum corresponds to (*circle one):*

A B C D E 3



ii) This spectrum corresponds to (*circle one):*

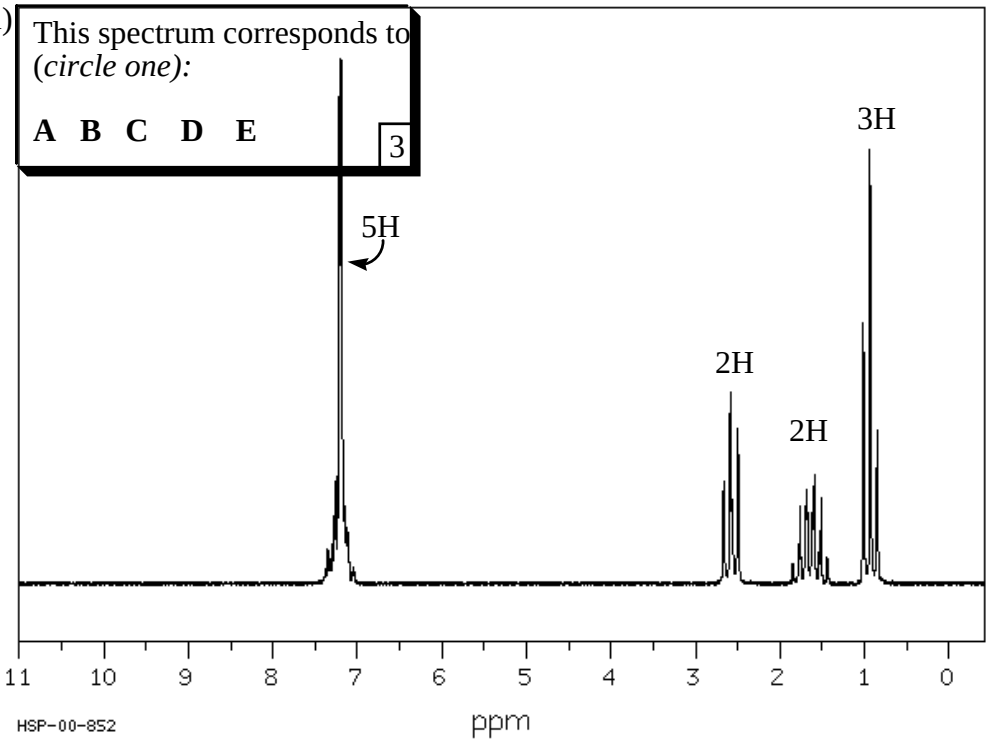
A B C D E 3



iii) This spectrum corresponds to (*circle one):*

A B C D E

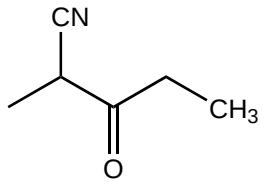
3



2. 2-butanol shows the base peak (highest intensity) in its mass spectrum at *m/z* = 45. Draw the molecular ion of 2-butanol ($M^{+\bullet}$) and the fragmentation mechanism that leads to this peak. Use these molecular masses in your calculations: C = 12; O = 16; H = 1.

3

3. Which of the following features would you **not** expect to see in the IR spectrum of the following molecule (*circle one)*?



a strong absorption at 1710 cm^{-1}

a medium absorption at 2250 cm^{-1}

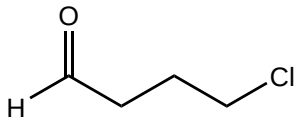
a strong absorption at 2900 cm^{-1}

a strong absorption at 3100 cm^{-1}

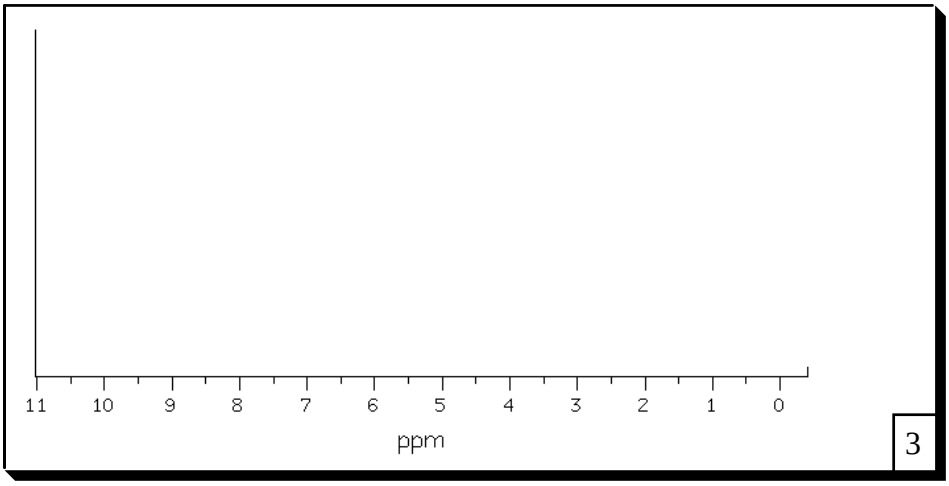
a medium absorption at 1465 cm^{-1}

1

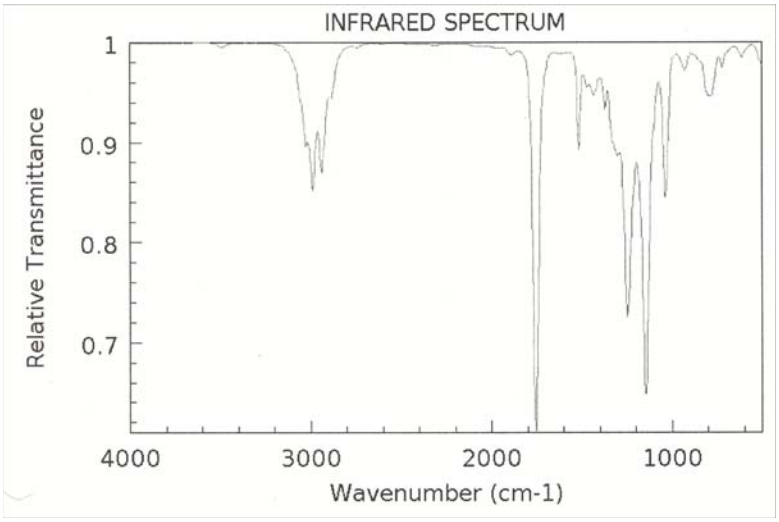
4. Draw an ^{1}H-NMR spectrum for 4-chlorobutanal (shown below). Estimate chemical shifts and draw proper splitting patterns. Draw a multiplet for any splitting > 6.

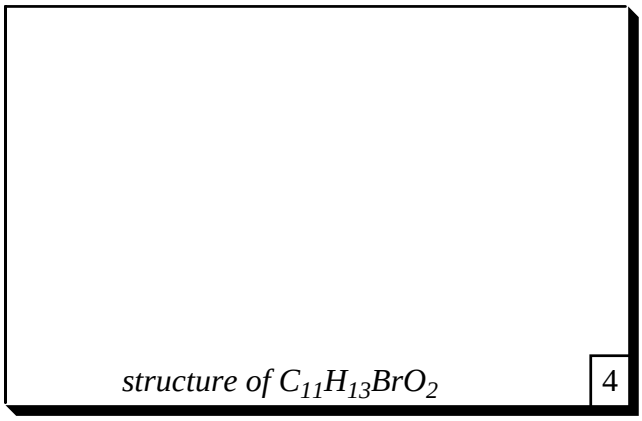


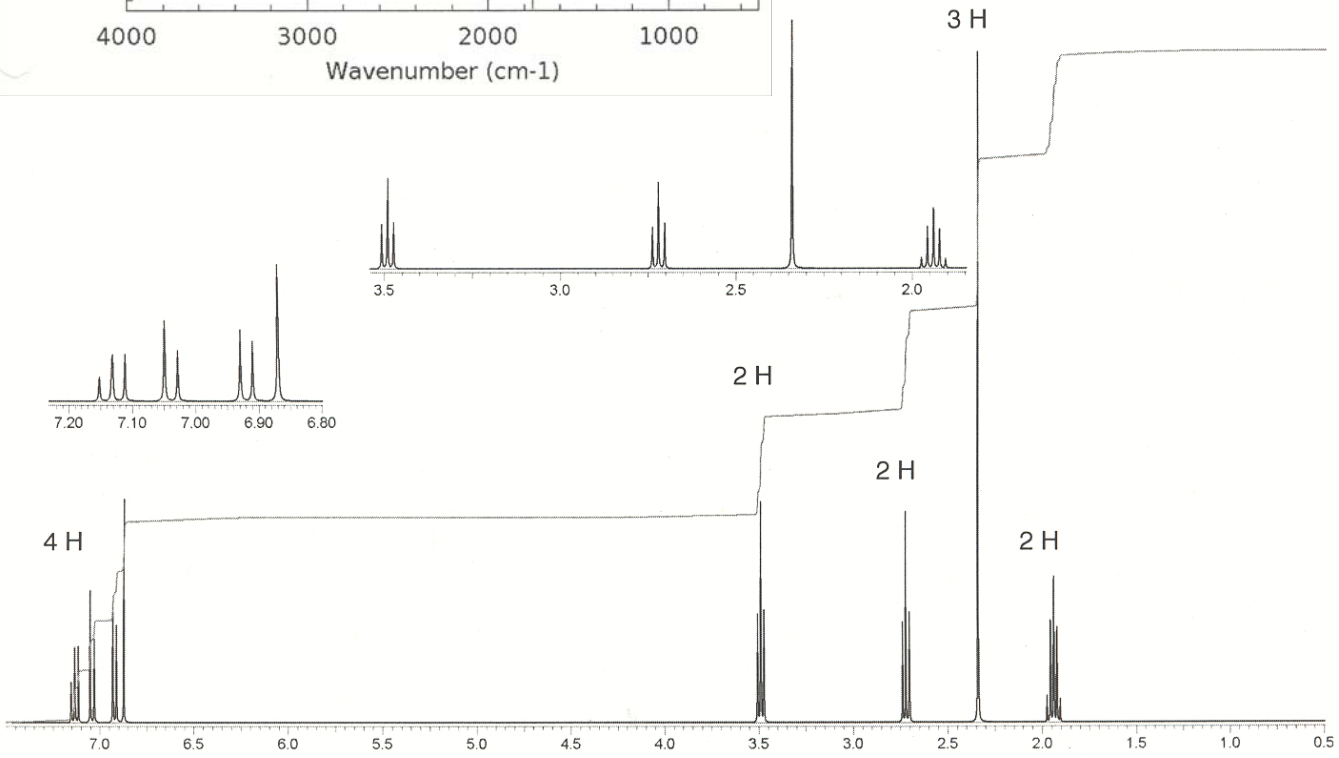
4-chlorobutanal



5. Use the following IR and ^{1}H-NMR spectra to deduce the structure of the proper $C_{11}H_{13}BrO_2$ isomer.







A Simplified Infrared Correlation Chart				
	Type of Vibration		**Frequency (cm^{-1})**	**Intensity**
C-H	Alkanes	(stretch)	3000-2850	s
	$-CH_3$	(bend)	1450 and 1375	m
	$-CH_2-$	(bend)	1465	m
	Alkenes	(stretch)	3100-3000	m
		(out-of-plane bend)	1000-650	s
	Aromatics	(stretch)	3150-3050	s
		(out-of-plane bend)	900-690	s
	Alkyne	(stretch)	~3300	s
	Aldehyde		2900-2800	w
			2800-2700	w
C-C	Alkane	not interpretatively useful		
C=C	Alkene		1680-1600	m-w
	Aromatic		1600 and 1475	m-w
C≡C	Alkyne		2250-2100	m-w
C=O	Aldehyde		1740-1720	s
	Ketone		1725-1705	s
	Carboxylic Acid		1725-1700	s
	Ester		1750-1730	s
	Amide		1670-1640	s
	Anhydride		1810 and 1760	s
	Acid Chloride		1800	s
C-O	Alcohols, Ethers, Esters, Carboxylic Acids, Anhydrides		1300-1000	s
O-H	Alcohols, Phenols			
	Free		3650-3600	m
	H-bonded		3500-3200	m
	Carboxylic Acids		3400-2400	m
N-H	Primary and Secondary Amines and Amides			
		(stretch)	3500-3100	m
		(bend)	1640-1550	m-s
C-N	Amines		1350-1000	m-s
C=N	Imines and Oximes		1690-1640	w-s
C≡N	Nitriles		2260-2240	m
X=C=Y	Allenes, Ketenes, Isocyanates, Isothiocyanates		2270-1950	m-s
N=O	Nitro ($R-NO_2$)		1550 and 1350	s
S-H	Mercaptans		2550	w
S=O	Sulfoxides		1050	s
	Sulfones, Sulfonyl Chlorides, Sulfates, Sulfonamides		1375-1300 and 1200-1140	s s
C-X	Fluoride		1400-1000	s
	Chloride		800-600	s
	Bromide, Iodide		<667	s