

Answer Key

Name: _____ Section _____

CHEM 226: Elementary Organic Chemistry
Spring 2013 Quiz 2:

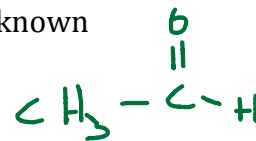
Chapter 12-Spectroscopy

Dr. Odago

1. An IR spectrum of an unknown organic molecule having the formula C_2H_4O reveals a strong absorption at $1715-1725\text{ cm}^{-1}$. To what class of compounds does the unknown belong?

C

- A) alcohol
B) amine
C) aldehyde
D) alkyne
E) ether



2. An IR spectrum of an unknown organic molecule having the formula C_3H_6O reveals a strong absorption at 1725 cm^{-1} . To what class of compounds does the unknown belong?

C

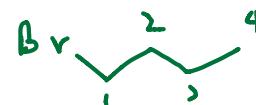
- A) acid chloride
B) alkene
C) ketone
D) alkyne
E) phenol



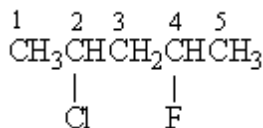
3. How many peak(s) would you expect to see in the 1H NMR spectrum of 1-bromobutane?

D

- A) 1
B) 2
C) 3
D) 4
E) more than 4



4. In the 1H NMR spectrum of the following molecule, the protons on which carbon will have the most downfield chemical shift?

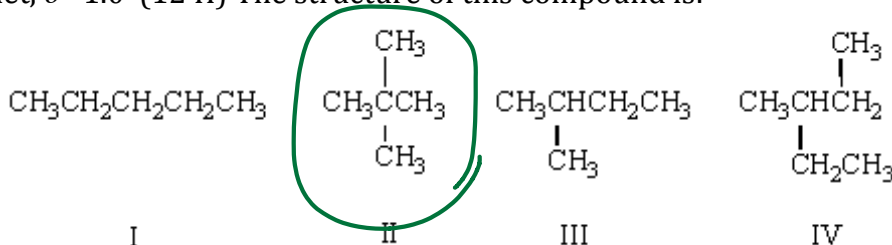


most electronegative
F, deshields, hence
more downfield

D

- A) 1
B) 2
C) 3
D) 4
E) 5

5. A compound with the molecular formula C_5H_{12} gave the following 1H NMR spectrum singlet, $\delta = 1.0$ (12 H) The structure of this compound is:

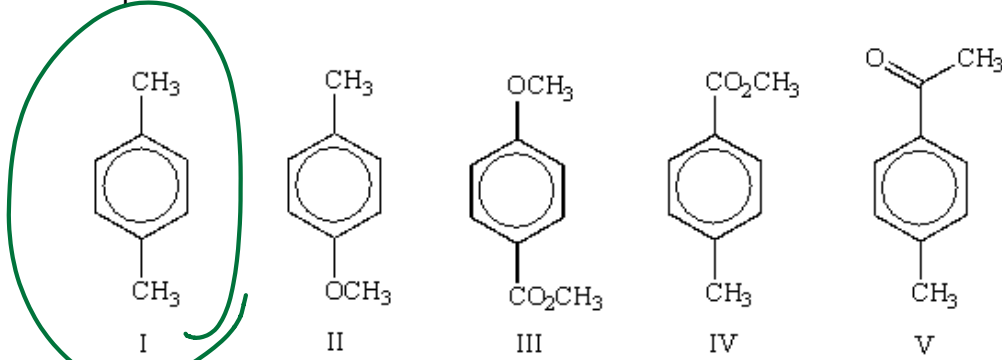


B

- A) I
B) II
C) III
D) IV
E) all are possible

all H equivalent

6. Which of the following molecules will show two peaks with an area ratio of 6:4 in its ^1H NMR spectrum?



- A) I
B) II
C) III

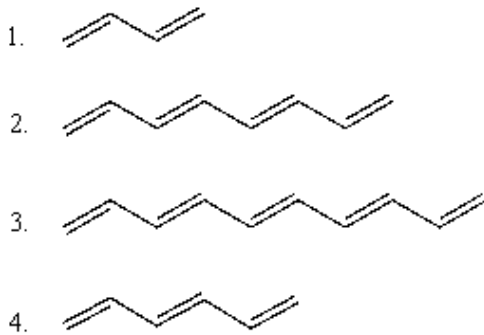
- D) IV
E) V

7. The compound will show what number of peaks in its ^1H decoupled ^{13}C NMR spectrum?

- A) 3
B) 4
C) 5

- D) 6
E) 9

8. The following compounds in order of increasing wavelength of maximum UV-VIS absorption are



- A) 1 < 2 < 3 < 4
B) 1 < 4 < 2 < 3
C) 3 < 2 < 4 < 1

- D) 4 < 3 < 2 < 1
E) 1 < 2 < 4 < 3

9. A bromoalkane shows two parent ion peaks m/z 122 and 124. What is the molecular formula?

- A) $\text{C}_4\text{H}_9\text{Br}$
B) $\text{C}_3\text{H}_7\text{Br}$
C) $\text{C}_2\text{H}_5\text{Br}$

- D) CH_3Br
E) $\text{C}_2\text{H}_{19}\text{Br}$

$$\text{C}_n\text{H}_{2n+1}\text{Br} = 124$$

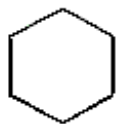
$$12n + 2n + 1 + 81 = 124 \quad \Rightarrow \quad \text{C}_3\text{H}_7\text{Br}^2$$

$$14n = 42$$

$$n = 3$$

10. Which of the following compounds will have one peak in its ^1H NMR and two peaks in its ^{13}C NMR spectrum?

A)



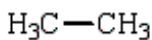
1 ^1H NMR peak
1 ^{13}C peak

B)



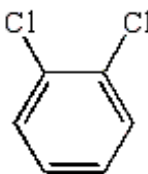
1 peak in both

C)



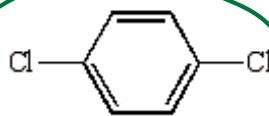
1 peak in both

D)



2 ^1H NMR peaks
3 ^{13}C NMR peaks

E)



1 ^1H peak
2 ^{13}C NMR peaks

E

Bonus Question

11. The ^1H NMR spectrum of two isomeric compounds with the molecular formula $\text{C}_2\text{H}_4\text{Cl}_2$ are shown. Predict the structures and match each with the correct spectrum based on the number of peaks, the chemical shift and/or the splitting pattern. (The peak at $\delta=0$ is due to TMS)

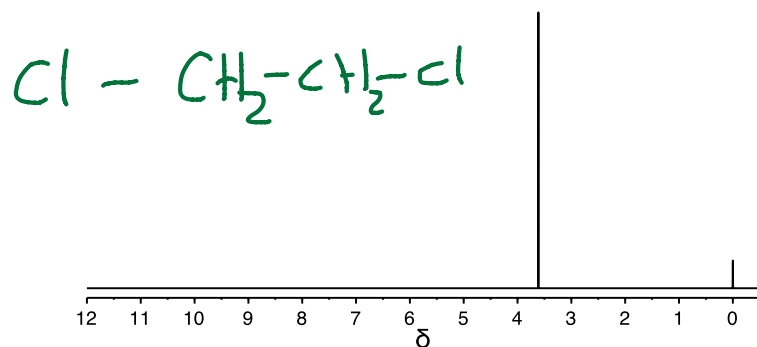
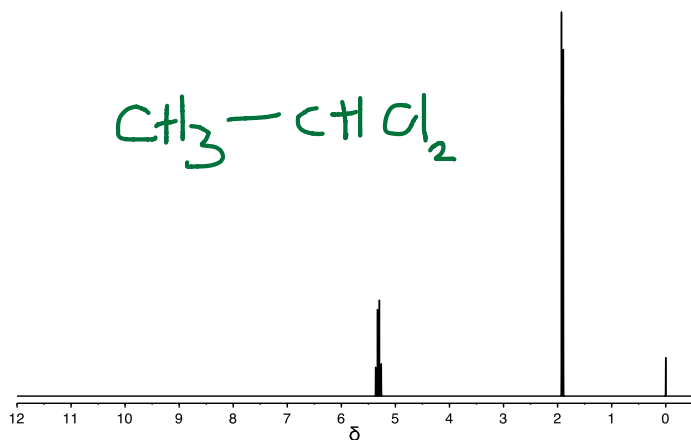


Table 12.2 Typical ^1H Chemical Shifts (Relative to Tetramethylsilane)

Type of ^1H	δ (ppm)	Type of ^1H	δ (ppm)
$\text{C}-\text{CH}_3$	0.85–0.95	$-\text{CH}_2-\text{F}$	4.3–4.4
$\text{C}-\text{CH}_2-\text{C}$	1.20–1.35	$-\text{CH}_2-\text{Br}$	3.4–3.6
		$-\text{CH}_2-\text{I}$	3.1–3.3
$\begin{array}{c} \text{C} \\ \\ \text{C}-\text{CH}-\text{C} \end{array}$	1.40–1.65	$\text{CH}_2=\text{C}$	4.6–5.0
$\text{CH}_3-\text{C}=\text{C}$	1.6–1.9	$-\text{CH}=\text{C}$	5.2–5.7
CH_3-Ar	2.2–2.5	$\text{Ar}-\text{H}$	6.6–8.0
$\begin{array}{c} \text{CH}_3-\text{C}=\text{O} \\ \end{array}$	2.1–2.6	$-\text{C}\equiv\text{C}-\text{H}$	2.4–2.7
$\text{CH}_3-\text{N} \begin{array}{l} \diagup \\ \diagdown \end{array}$	2.1–3.0	$\begin{array}{c} \text{O} \\ \\ -\text{C}-\text{H} \end{array}$	9.5–9.7
$\text{CH}_3-\text{O}-$	3.5–3.8	$\begin{array}{c} \text{O} \\ \\ -\text{C}-\text{OH} \end{array}$	10–13
$-\text{CH}_2-\text{Cl}$	3.6–3.8	$\text{R}-\text{OH}$	0.5–5.5
$-\text{CHCl}_2$	5.8–5.9	$\text{Ar}-\text{OH}$	4–8

Table 12.4 Infrared Stretching Frequencies of Some Typical Bonds

Bond type	Group	Class of compound	Frequency range (cm^{-1})
single bonds to hydrogen	$\text{C}-\text{H}$	alkanes	2850–3000
	$=\text{C}-\text{H}$	alkenes and aromatic compounds	3030–3140
	$\equiv\text{C}-\text{H}$	alkynes	3300
	$\text{O}-\text{H}$	alcohols and phenols	3500–3700 (free) 3200–3500 (hydrogen-bonded)
	$\text{O}-\text{H}$	carboxylic acids	2500–3000
double bonds	$\text{N}-\text{H}$	amines	3200–3600
	$\text{S}-\text{H}$	thiols	2550–2600
	$\text{C}=\text{C}$	alkenes	1600–1680
	$\text{C}=\text{N}$	imines, oximes	1500–1650
triple bonds	$\text{C}=\text{O}$	aldehydes, ketones, esters, acids	1650–1780
	$\text{C}\equiv\text{C}$	alkynes	2100–2260
	$\text{C}\equiv\text{N}$	nitriles	2200–2400