First name:_____Last name:_____
i.d. (last 4 digits only):_____

Midterm 1

Version 1

Organic Chemistry 2

CHEM222 and CHEM234

29 January 2014, 6:15-9:00 pm

INSTRUCTIONS:

Please write your **Name and ID number** in the space provided above.

This is a Closed Book Examination. Multiple choice questions **1-8** are worth **2 points** each and **9-30** are worth **3 points** each. Short answer questions **31-36** are worth **3 points** each.

Answer multiple choice questions on the answer sheet provided (scantron) with a pen or pencil and short answer questions directly on the exam paper with ink.

Molecular models and pen/pencils are allowed.

Calculators, dictionaries or electronic devices are NOT allowed.

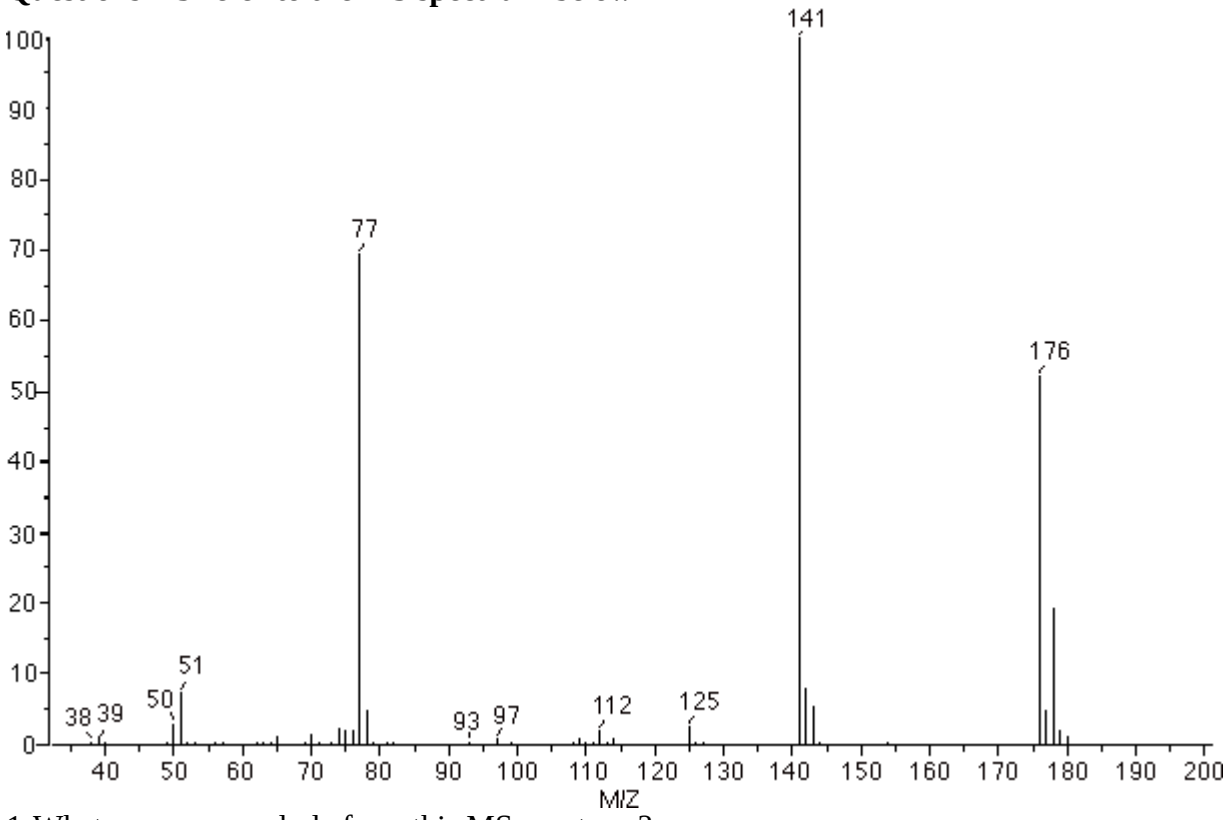
At the end you must **hand in ALL pages** of your exam.

McGill University values academic integrity. Therefore all students must understand the meaning and consequences of cheating, plagiarism, and other academic offenses under the code of students conduct and disciplinary procedures.

Good Luck!

ANSWER QUESTION 1-30 ON THE SCANTRON (multiple answer sheet). Keep in mind that the scantron will NOT be returned to students.

Questions 1-3 refer to the MS spectrum below



1-What can you conclude from this MS spectrum?

a) this molecule contains Br
b) this molecule contains Cl
c) this molecule contains no F
d) this molecule contains an odd number of N

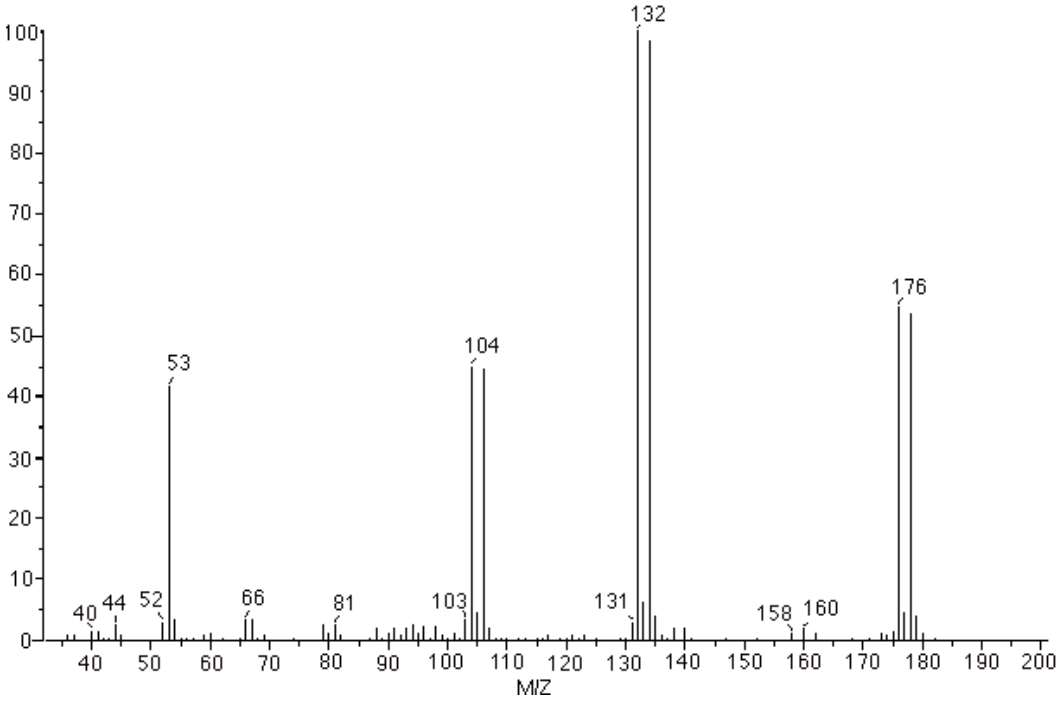
2-Which of the peaks of the above MS spectrum corresponds to the base peak?

a) 141
b) 176
c) 180
d) Does not show up

3- In the MS spectrum above, what is the peak at 177?

a) an impurity
b) it is a fragment
c) it is the molecular ion
d) it is the molecule with one ^{13}C

Questions 4, 5 and 6 refer to the MS spectrum below



4- Which of the peaks of the above MS spectrum corresponds to the molecular ion?

a) 132
b) 176
c) 178
d) 180

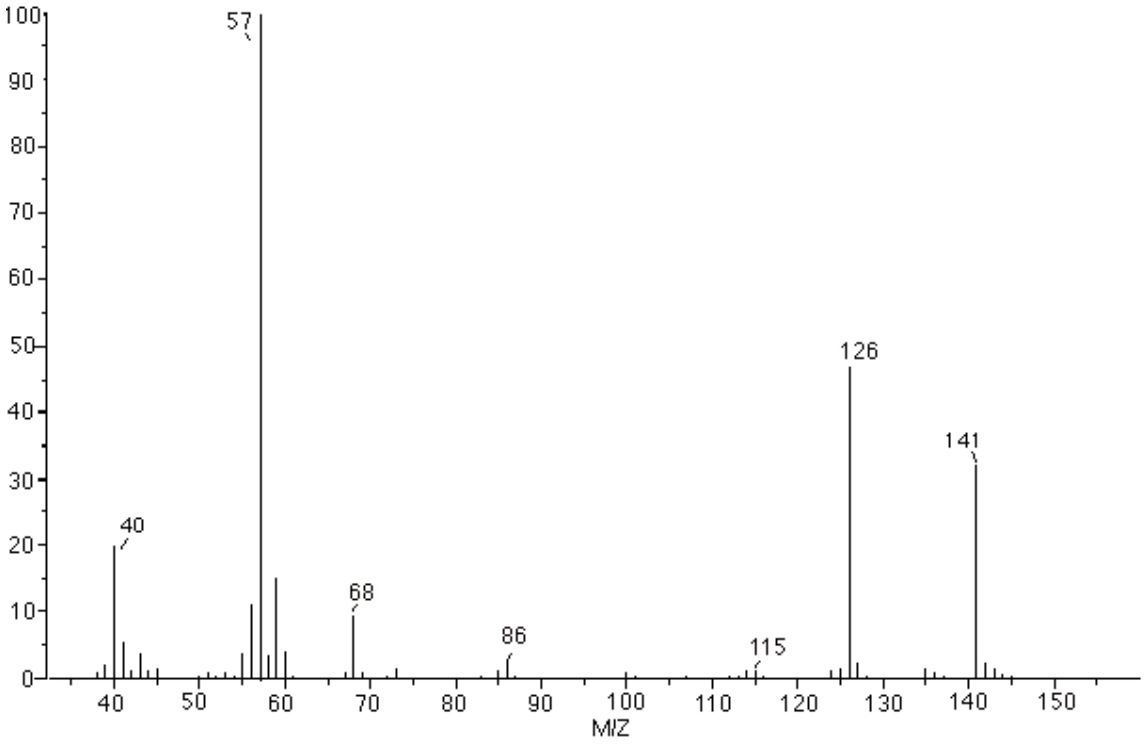
5- What can you say about the molecule that gives the MS spectrum above?

a) it contains two chlorine atoms
b) it contains nitrogen
c) it contains bromine
d) it contains an anhydride

6- In the MS spectrum above, what is the peak at 179?

a) it is the molecular ion ($M^{\bullet +}$)
b) it is caused by nitrogen
c) it is caused by ^{13}C
d) it is caused by both ^{81}Br and ^{13}C

7-What can you say about the molecule that gives the MS spectrum below?



a) it contains bromine
b) it contains chlorine
c) it contains nitrogen
d) it contains sulfur

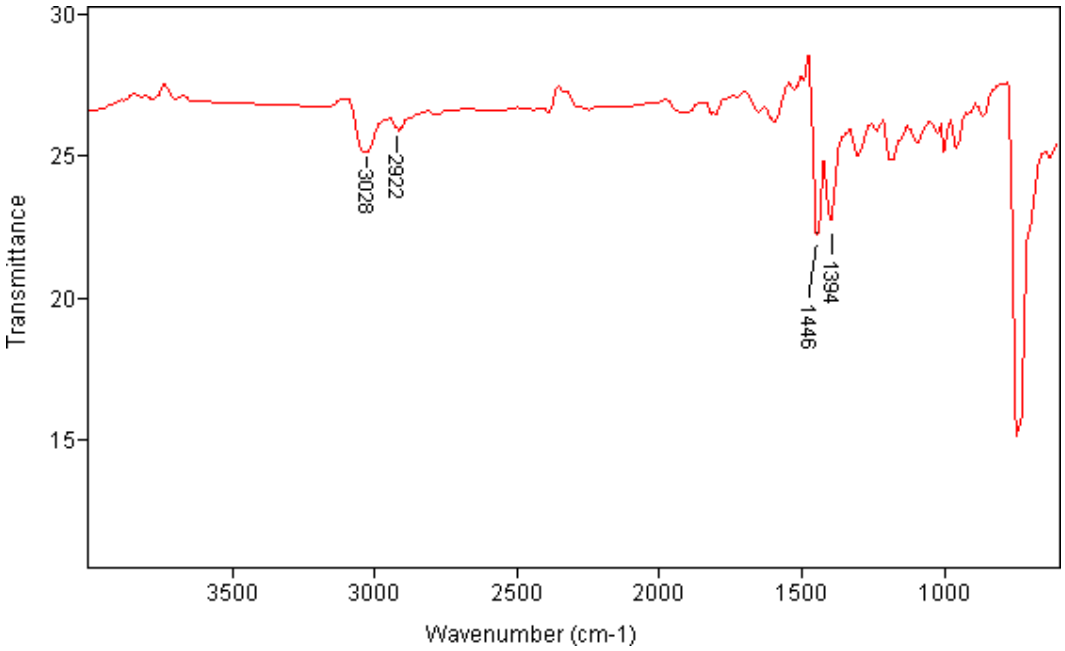
8- What is the even electron rule useful for?

a) To differentiate the strongest signals in IR
b) To figure out if the molecule contains halogens in MS
c) To determine if the molecular ion is showing up in MS
d) To find out if the molecules contains oxygen

9- Which of the following types of bonds are <u>NOT</u> easy to distinguish by IR?

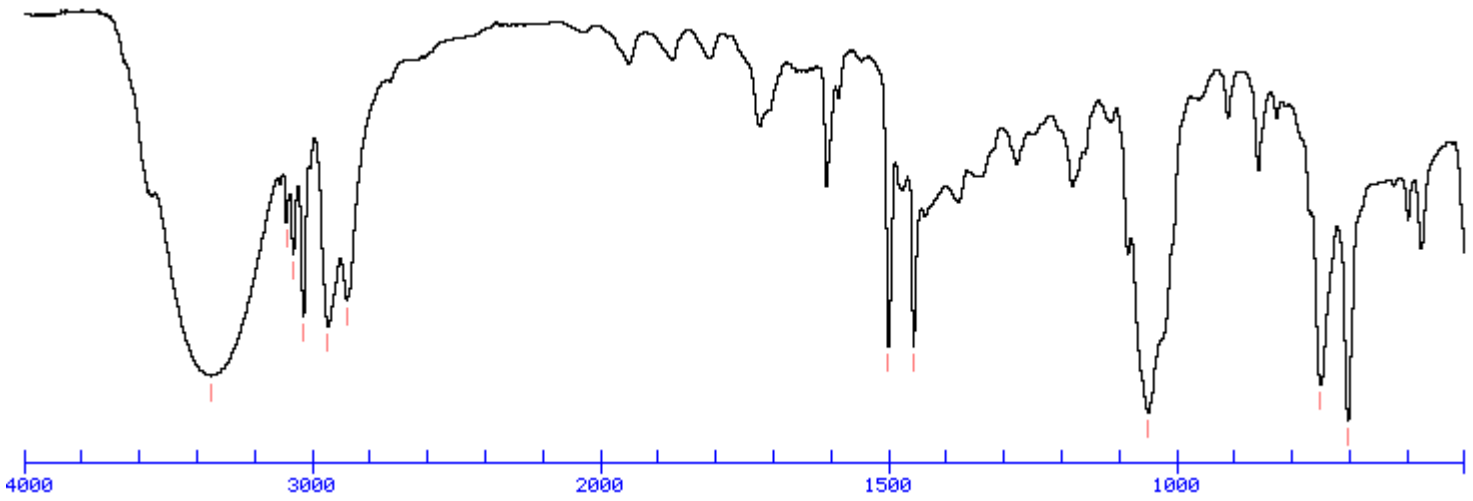
a) C-Br
b) O-H
c) carbonyls
d) triple bonds

10- From the IR spectrum below, what can you conclude?



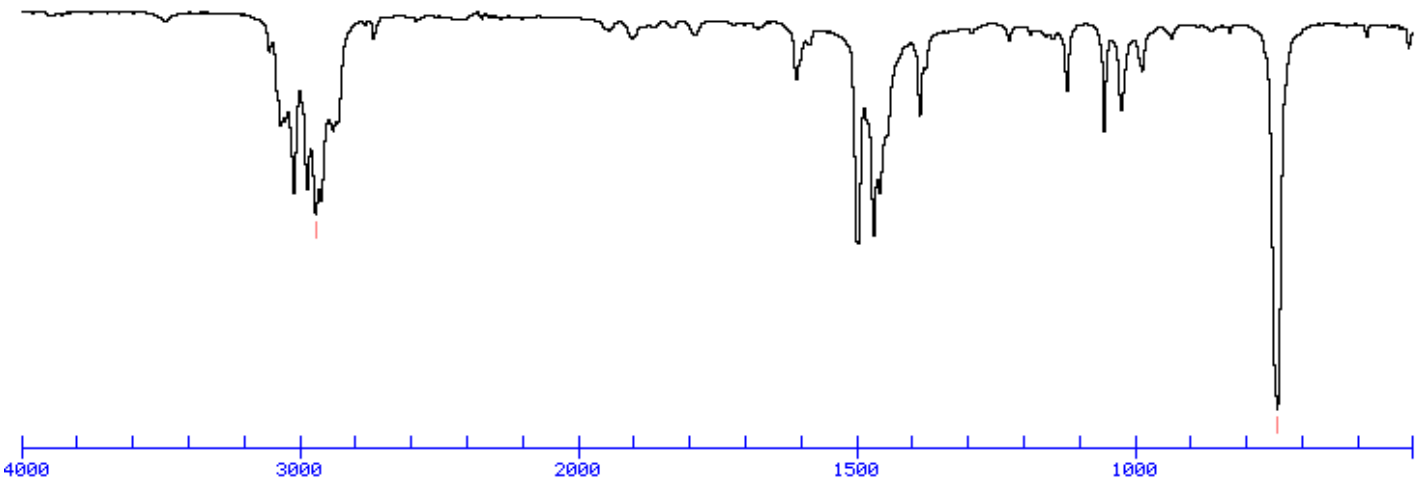
a) presence of an ester
b) presence of an alcohol
c) presence of a triple bond
d) absence of an amine

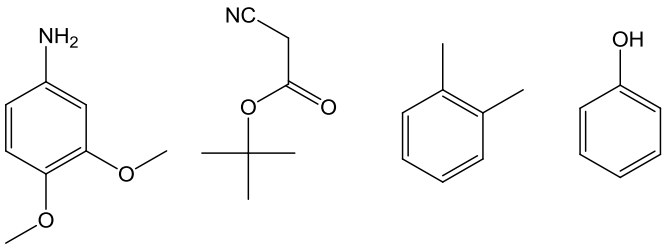
11- Which of the statements below is <u>WRONG</u> about this IR spectrum:



a) presence of an alcohol
b) presence of an aromatic ring
c) absence of a ketone
d) absence of sp^3 C-H bonds

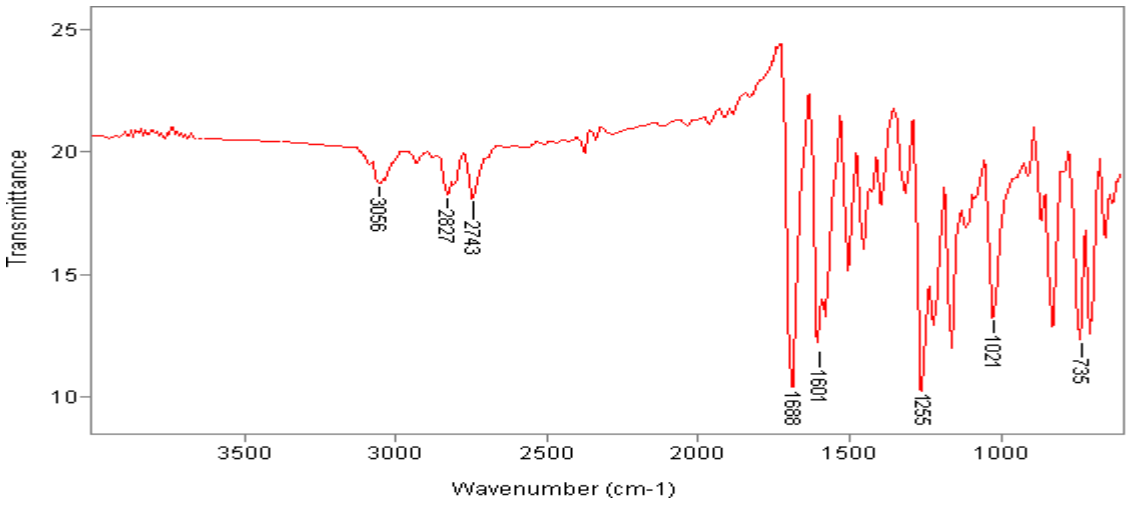
12- What is the most likely molecule giving rise to the IR spectrum below?

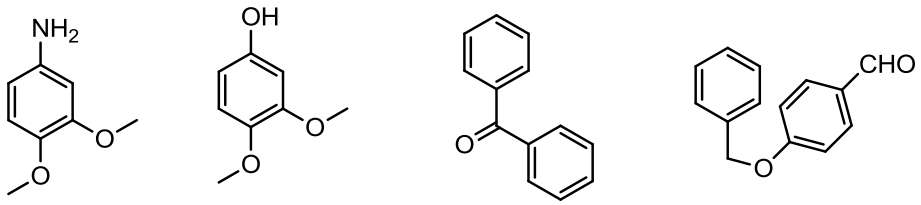




a) b) c) d)

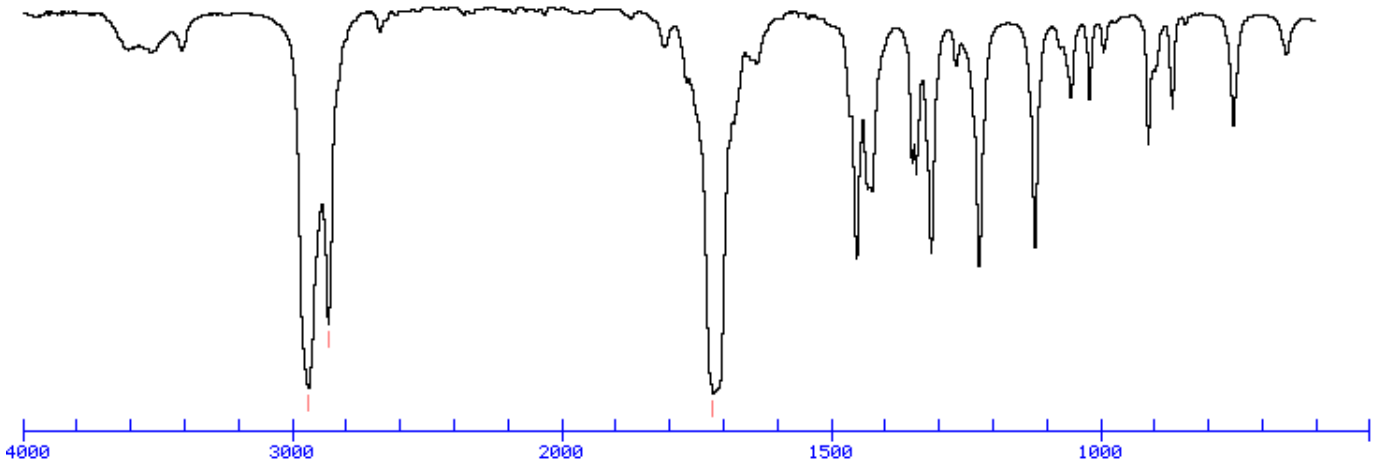
13- What is the most likely molecule giving rise to the IR spectrum below?

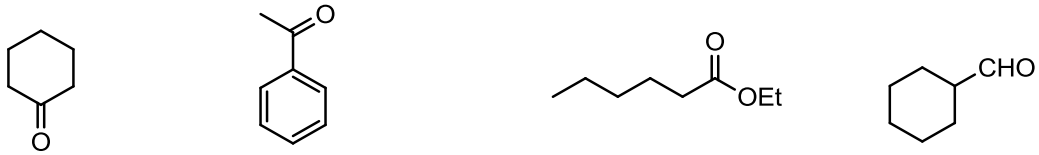




a) b) c) d)

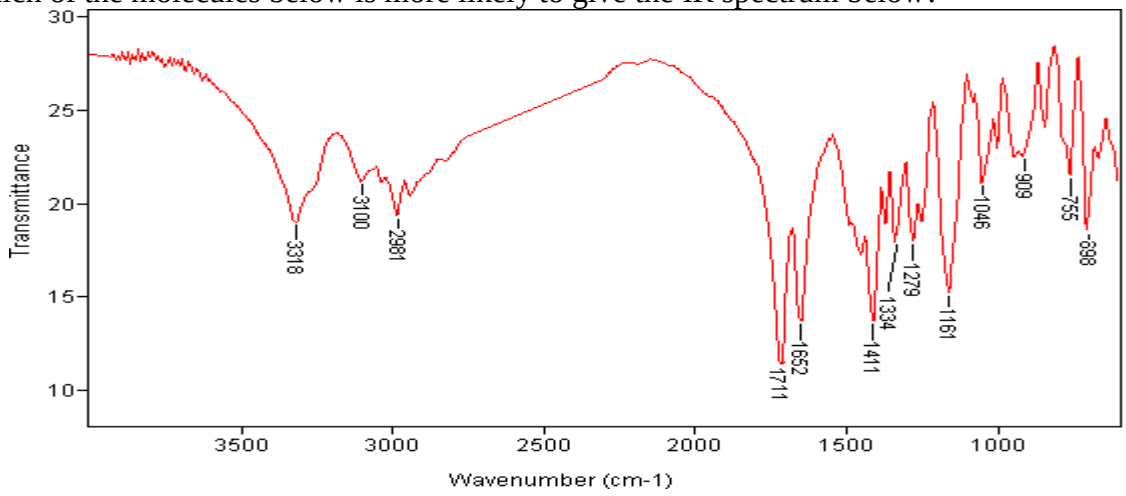
14-Which of the molecules below is more likely to give the IR spectrum below?

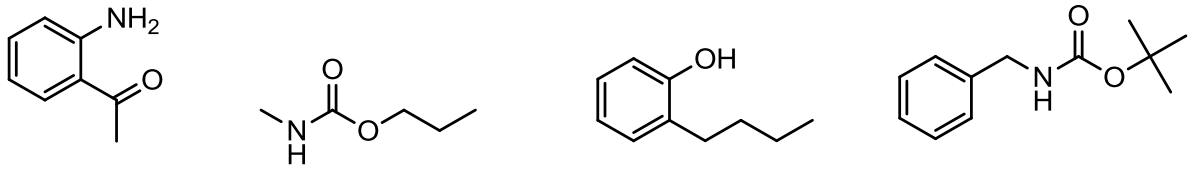




a) b) c) d)

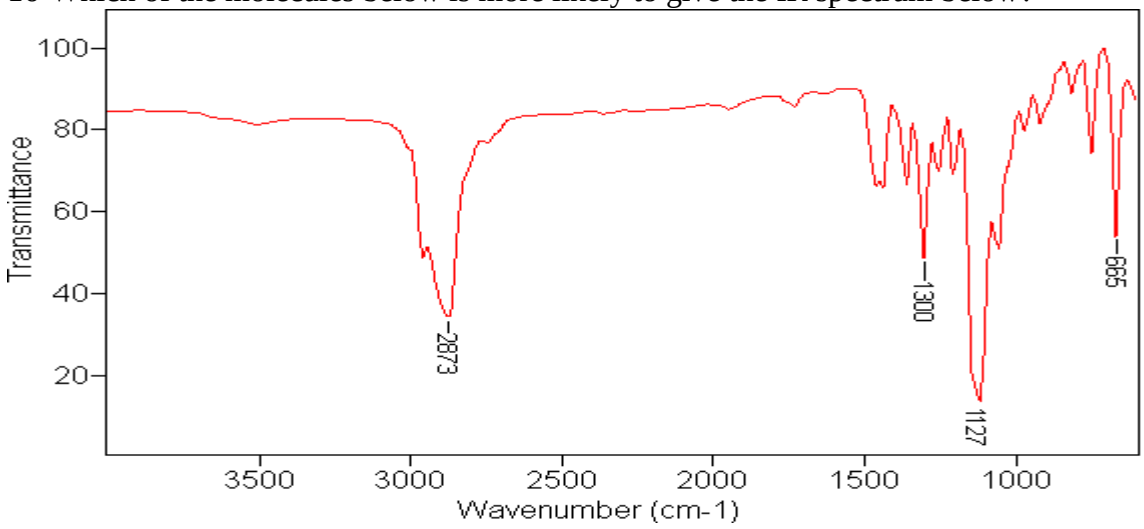
15-Which of the molecules below is more likely to give the IR spectrum below?

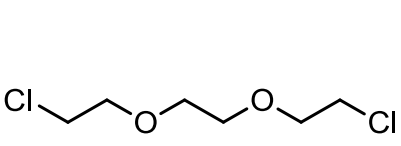




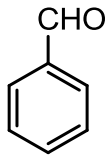
a) b) c) d)

16-Which of the molecules below is more likely to give the IR spectrum below?

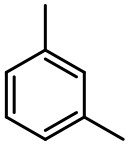




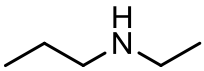
a)



b)

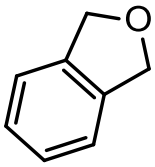


c)



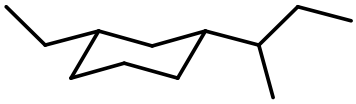
d)

17- How many **^{1}H** NMR signals are theoretically expected for the molecule below?



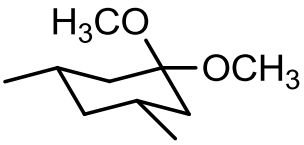
a) 2
b) 3
c) 4
d) 5

18- How many **^{1}H** NMR signals would you expect for the molecule below?



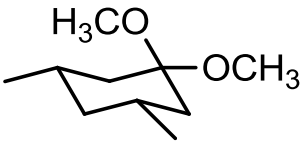
a) 11
b) 15
c) 17
d) 18

19- How many **^{1}H** NMR signals would you expect for the molecule below?



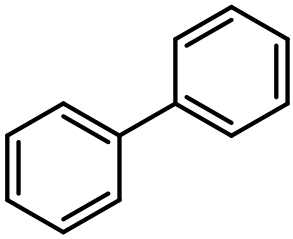
a) 5
b) 6
c) 8
d) 11

20- How many **^{13}C** NMR signals would you expect for the molecule below?



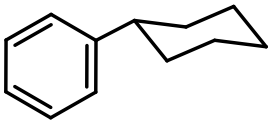
a) 5
b) 6
c) 7
d) 9

21- How many ^{13}**C** NMR signals would you expect for the molecule below?



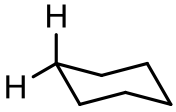
a) 3
b) 4
c) 6
d) 8

22- How many ^{13}**C** NMR signals would you expect for the molecule below?



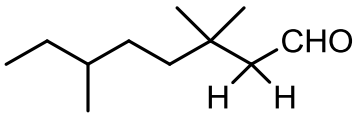
a) 7
b) 8
c) 10
d) 11

23-How do you qualify the two protons drawn out in the molecule below?



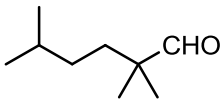
a) homotopic
b) enantiotopic
c) diastereotopic
d) none of the above

24-How can you qualify the two protons drawn out in the molecule below?

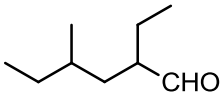


a) homotopic
b) enantiotopic
c) diastereotopic
d) none of the above

25- Which of the molecules below is expected to give a ^{1}H NMR spectrum with 12 signals?

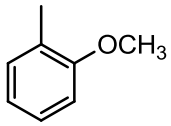


a)



b)

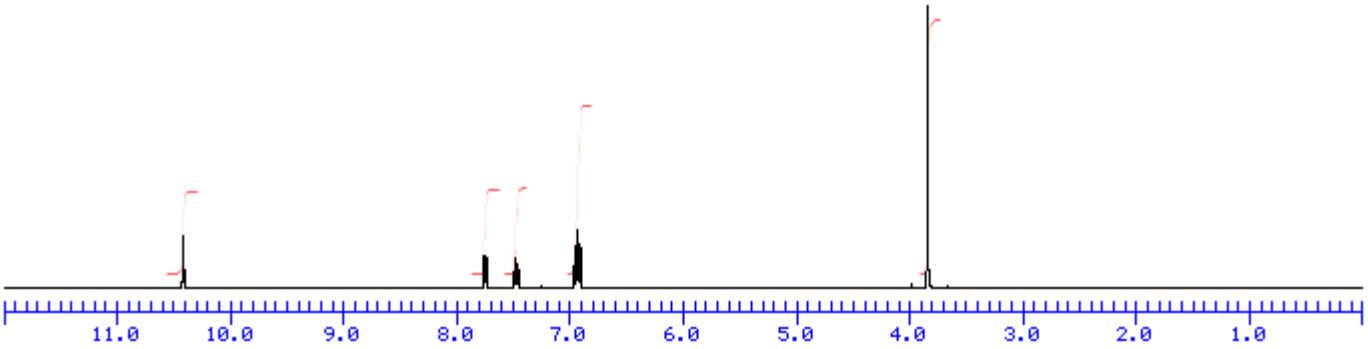
c)



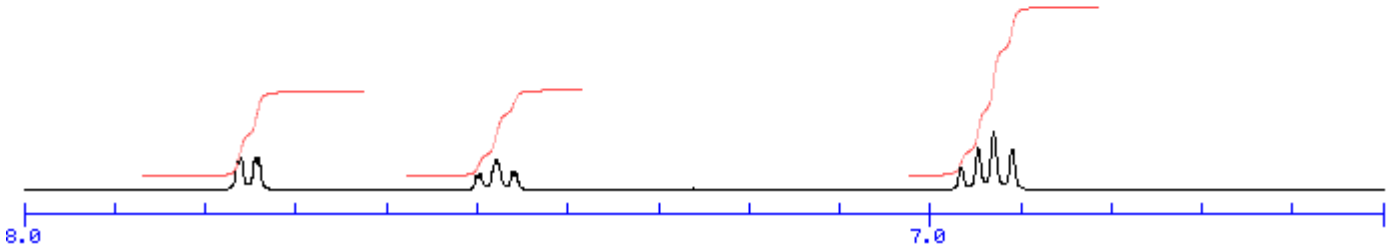
d)

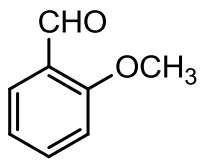
26- Which of the molecules below is more likely to have resulted in the ^{1}H NMR spectrum shown?

FULL SPECTRUM

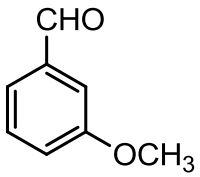


EXPANSION

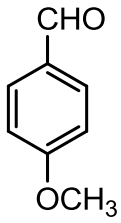




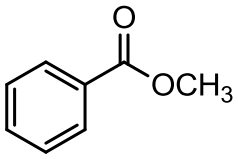
a)



b)



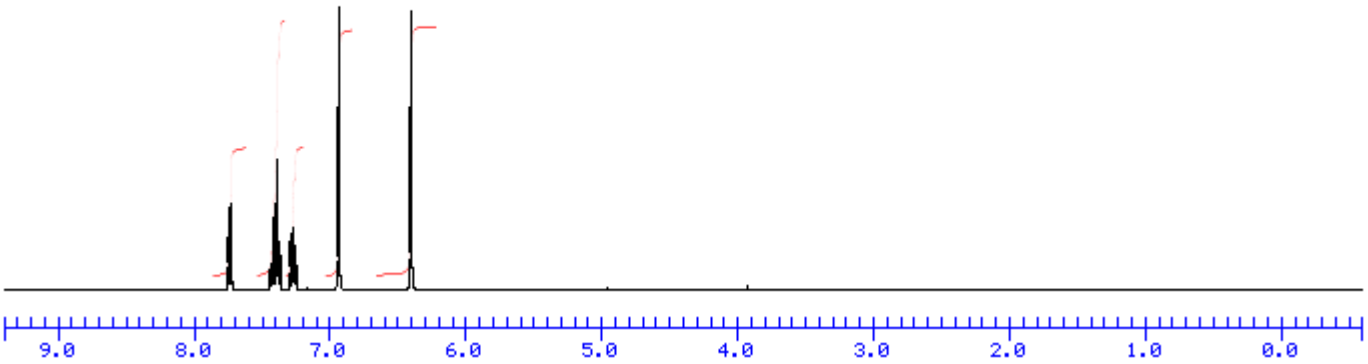
c)



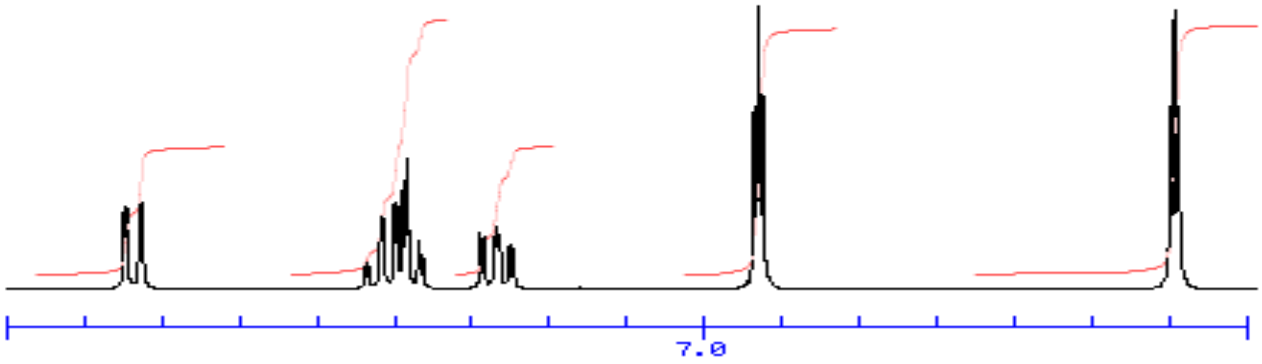
d)

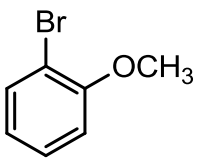
27- Which of the molecules below is more likely to have resulted in the ^{1}H NMR spectrum shown (expansions are shown)?

FULL SPECTRUM

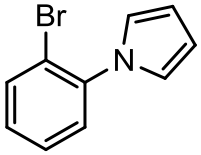


EXPANSION

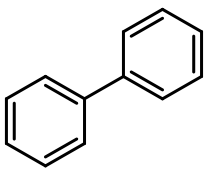




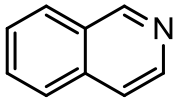
a)



b)

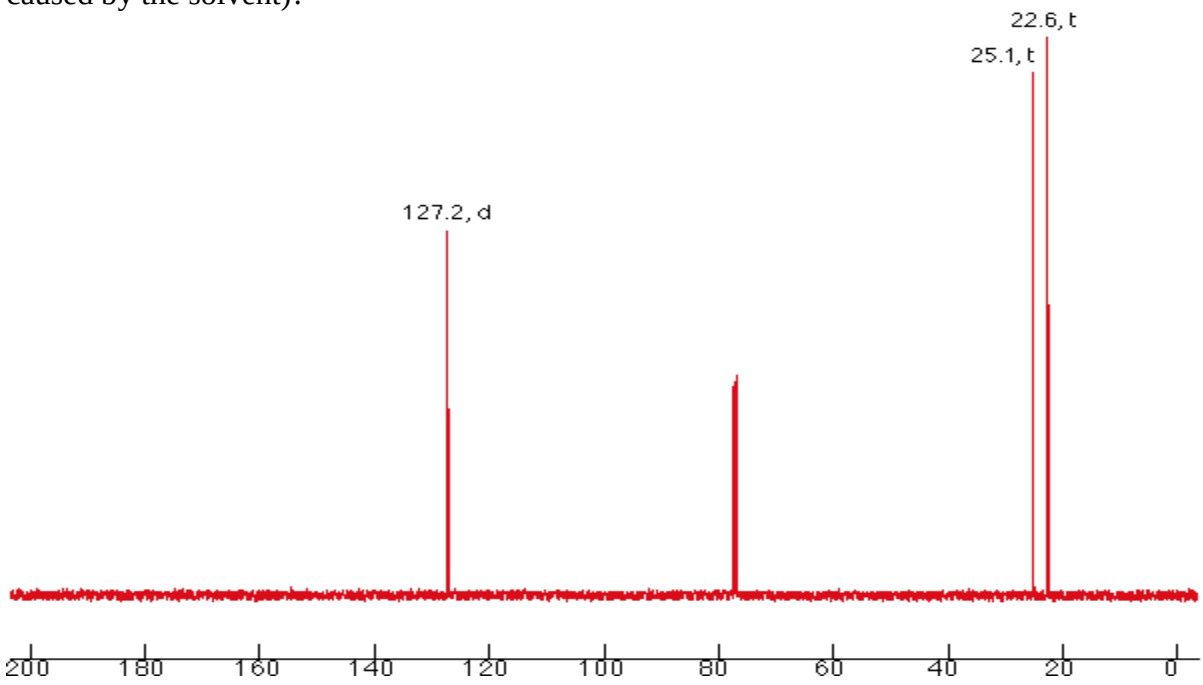


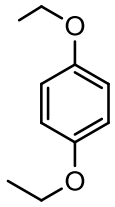
c)



d)

28- Which of the molecules below could best account for the ^{13}C NMR spectrum shown (triplet at 77 ppm is caused by the solvent)?

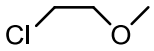




a)

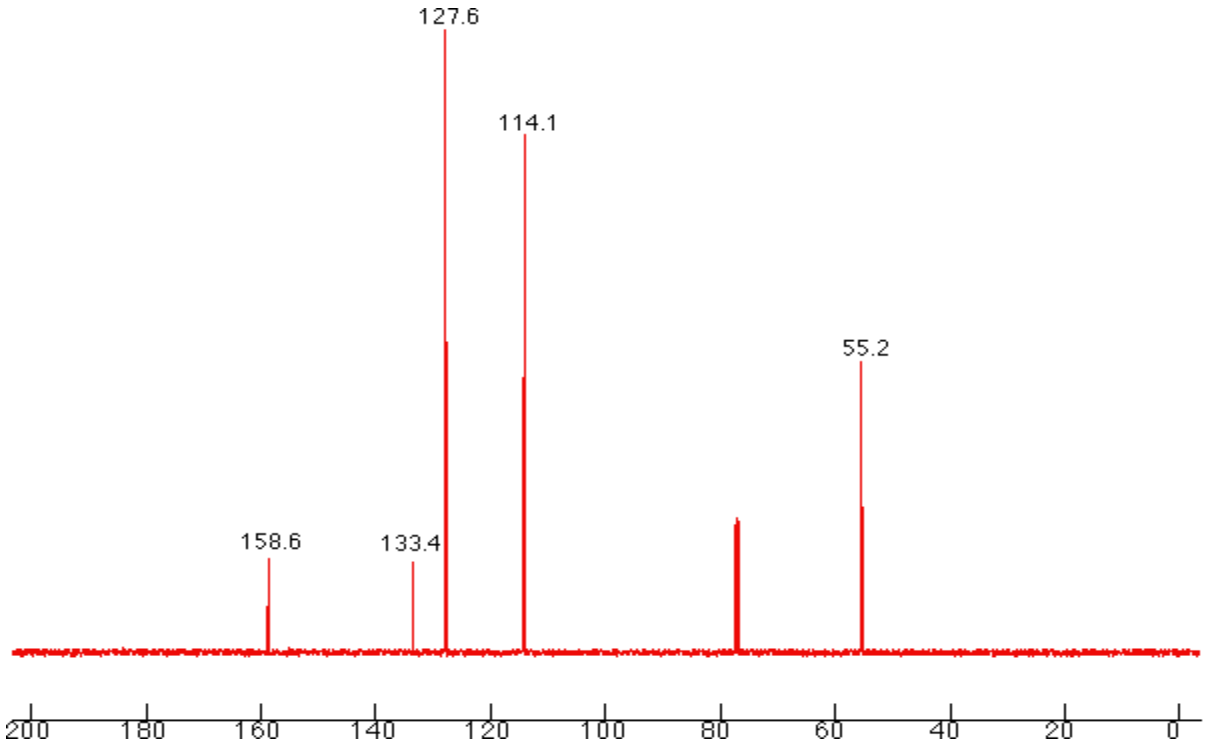
b)

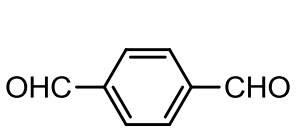
c)



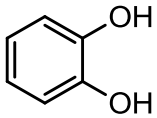
d)

29- Which of the molecules below could best account for the ^{13}C NMR spectrum shown?
(triplet at 77 ppm is caused by solvent)

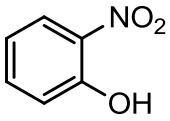




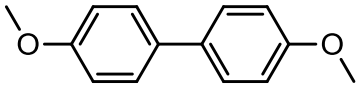
a)



b)



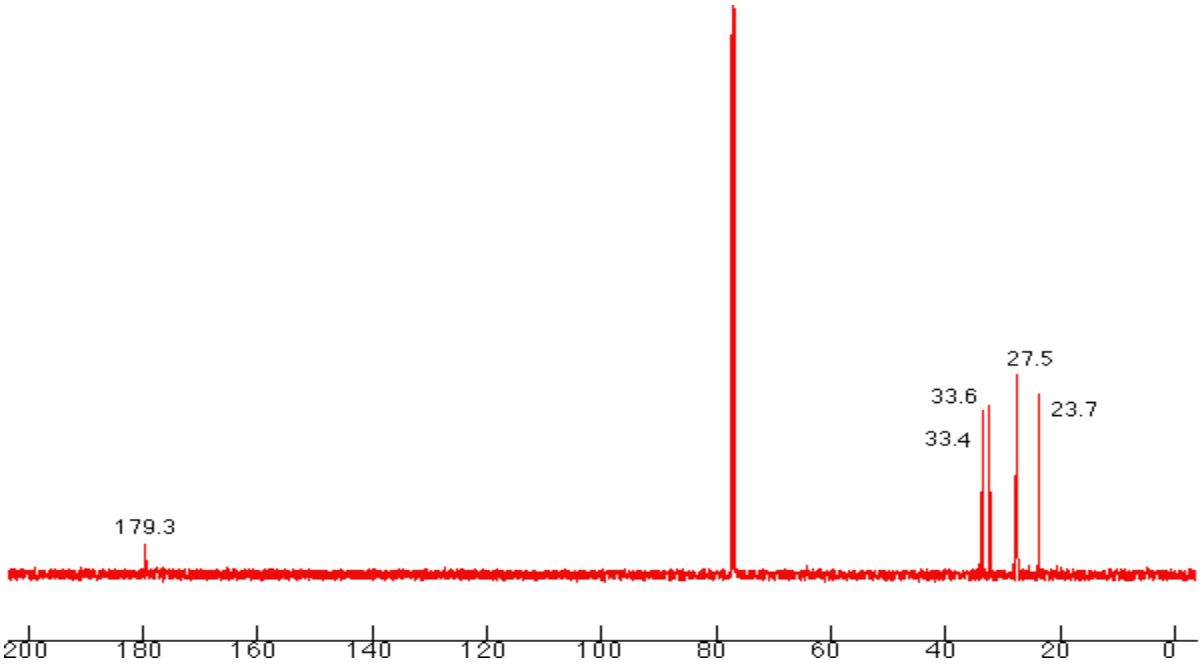
c)

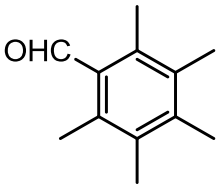


d)

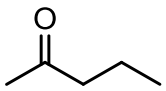
30- Which of the molecules below could best account for the ^{13}C NMR spectrum shown?
(the signal at ~77 ppm is due to the NMR solvent)

FULL SPECTRUM

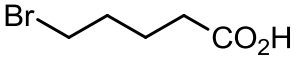




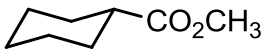
a)



b)



c)

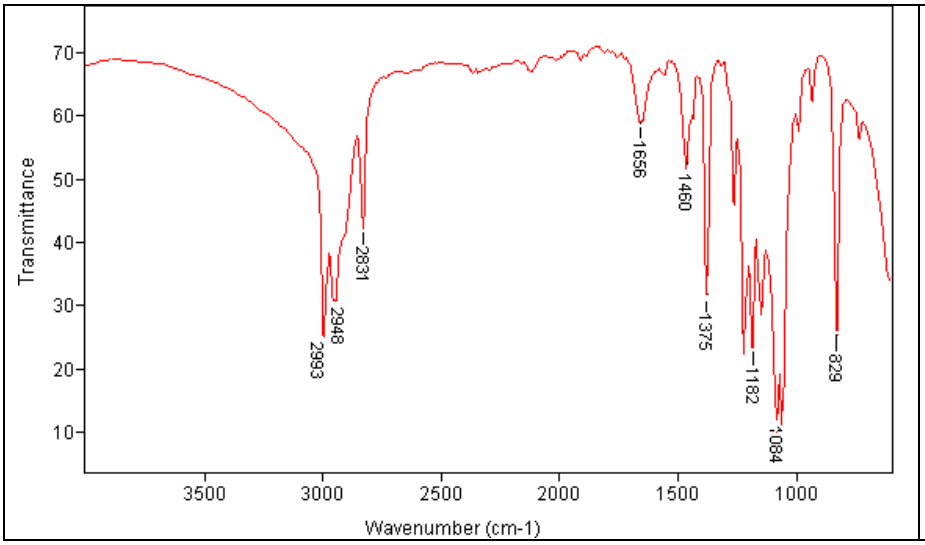


d)

FOR QUESTIONS 30-36, ANSWER DIRECTLY IN THE BOX PROVIDED
ANY STRUCTURES OUTSIDE THE BOX WILL NOT BE CONSIDERED BY THE GRADERS.

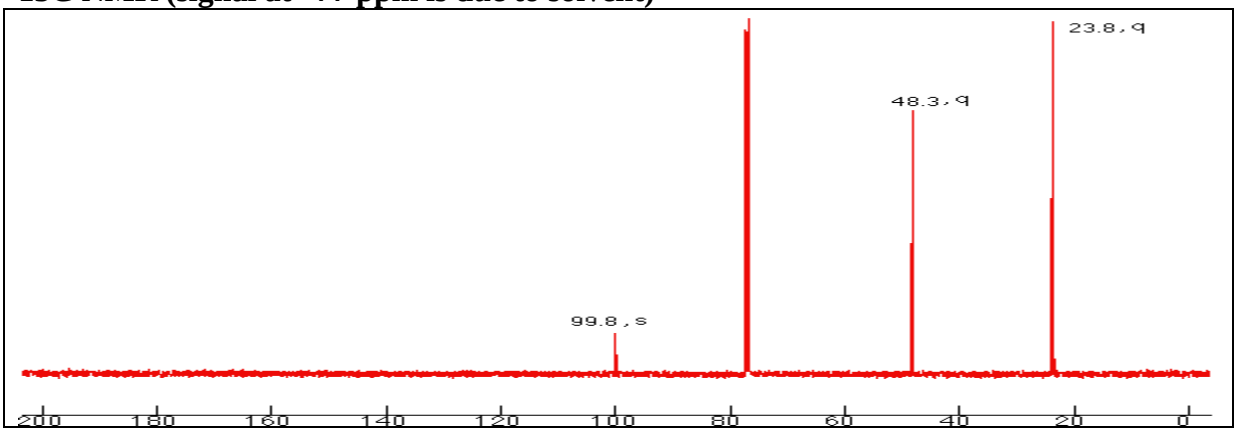
31- Spectra are shown for a molecule of formula **$C_5H_{12}O_2$.** Propose a structure (write final answer in the box).

IR

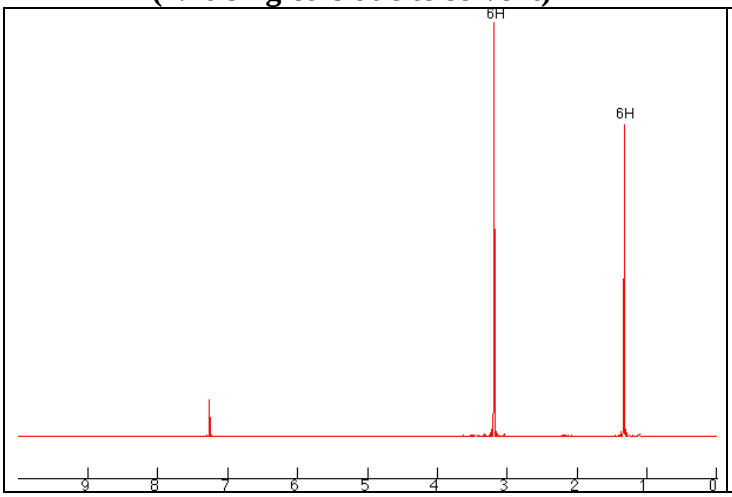


ANSWER

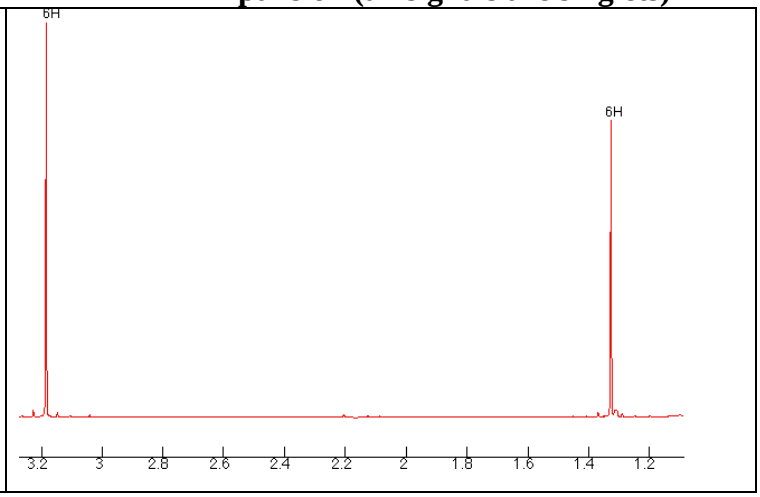
13C NMR (signal at ~77 ppm is due to solvent)



1H NMR (7.26 singlet is due to solvent)

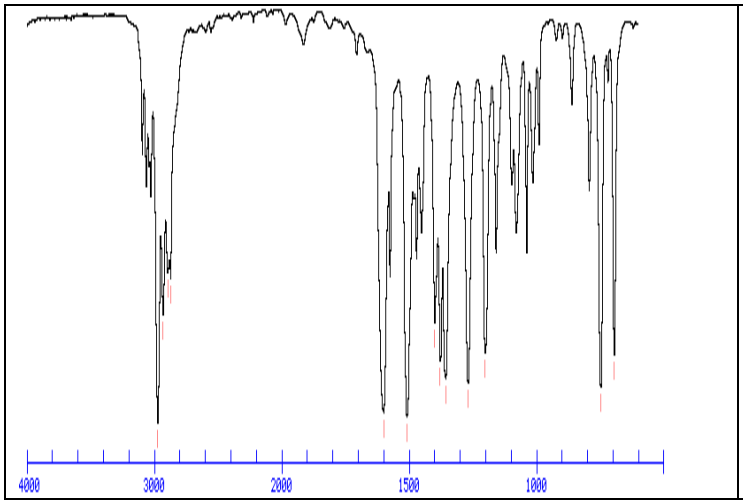


1H NMR Expansion (all signals are singlets)

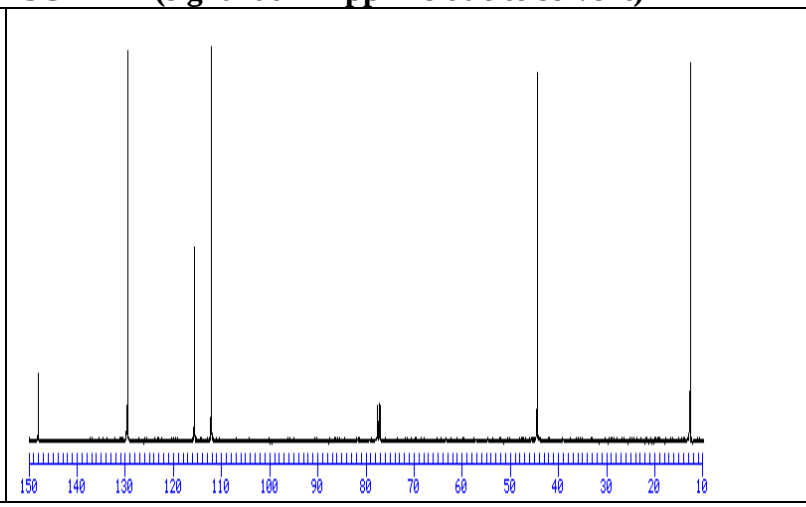


32- Spectra are shown for a molecule of formula **$C_{10}H_{15}N$.** Propose a structure (write final answer in the box).

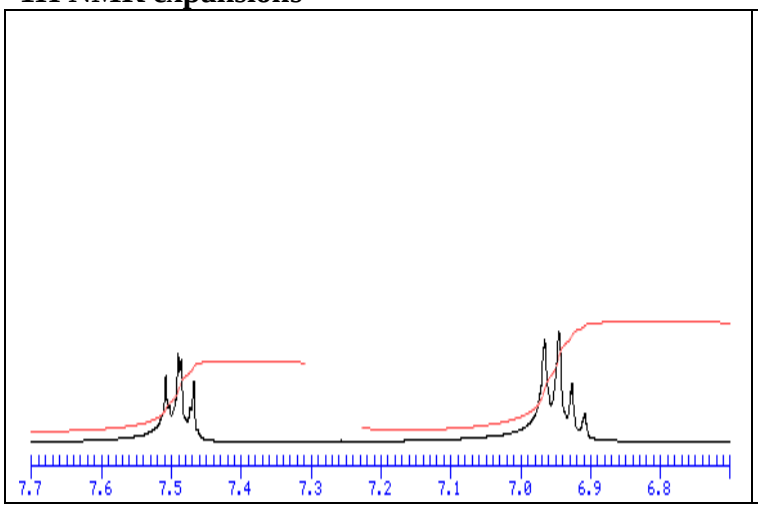
IR

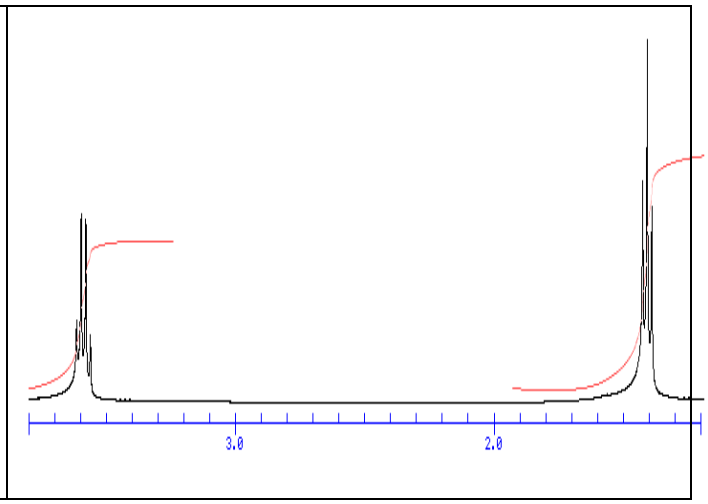


13C NMR (signal at ~77 ppm is due to solvent)

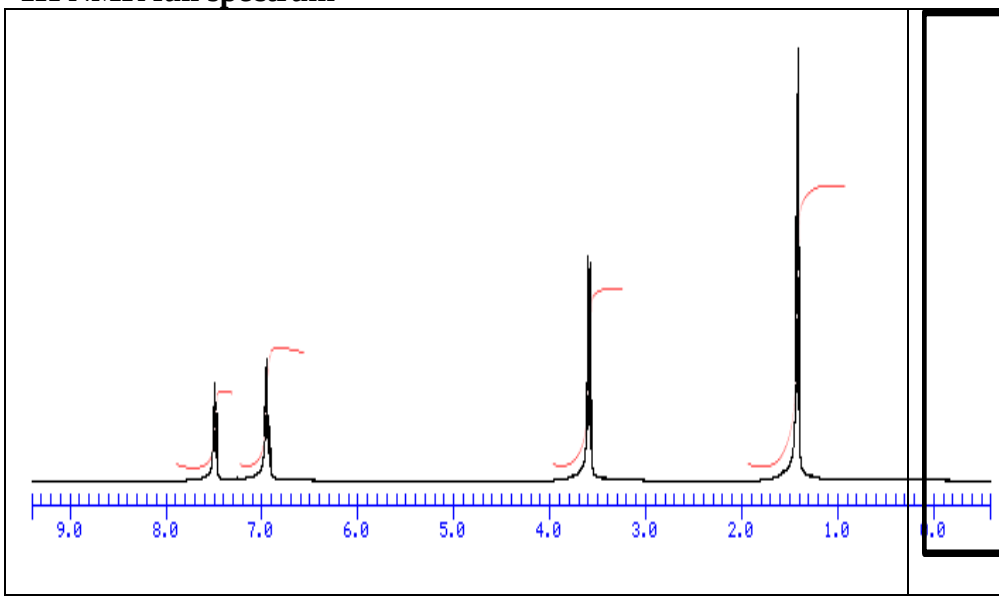


1H NMR expansions





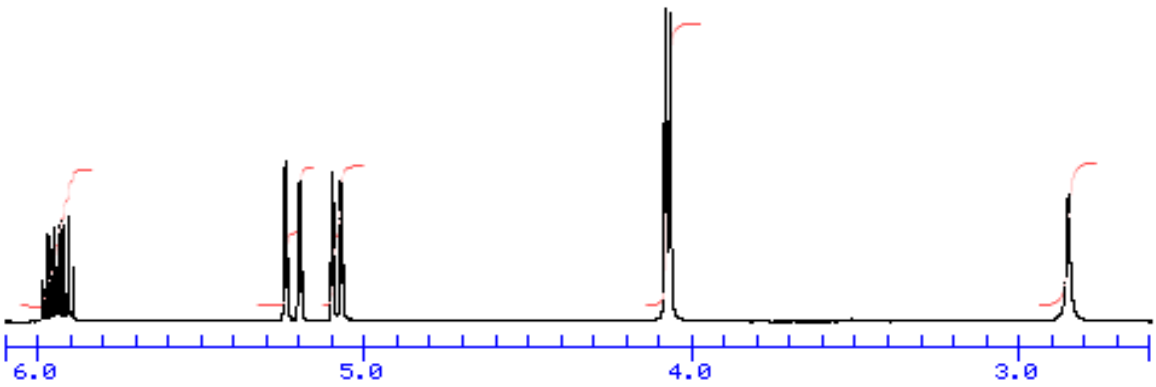
1H NMR full spectrum



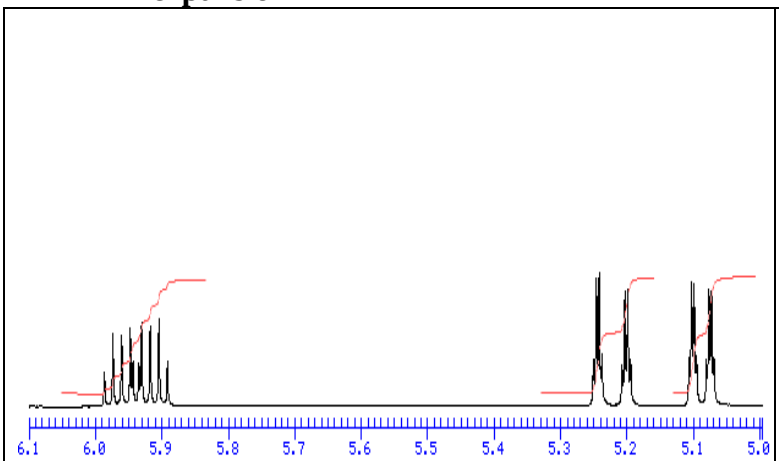
ANSWER

33- Spectra are shown for a molecule of formula **C_3H_6O.** Propose a structure (write final answer in the box).

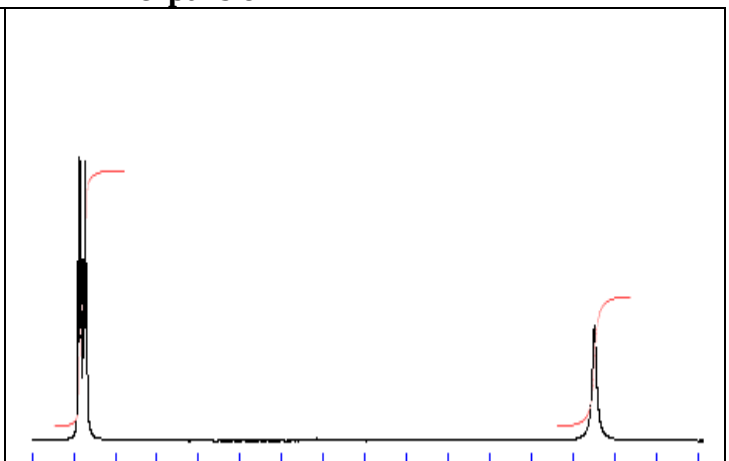
1H NMR (showing only the area with signals)



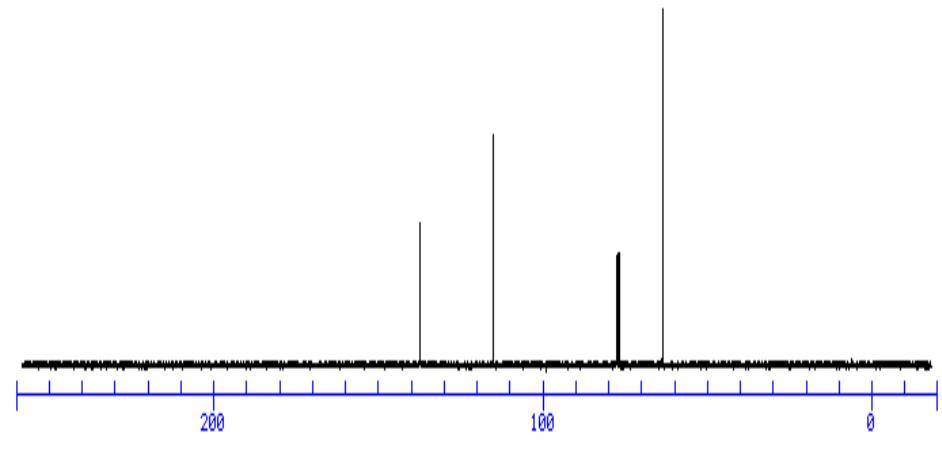
1H NMR expansion



1H NMR expansion



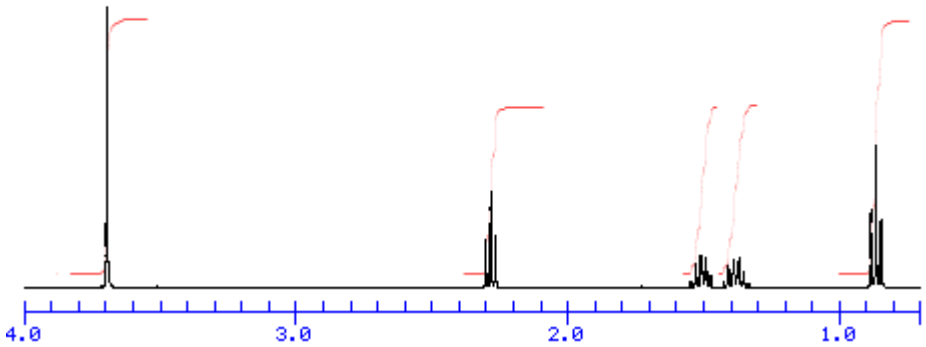
13CNMR (thick signal at ~77 ppm is caused by solvent)



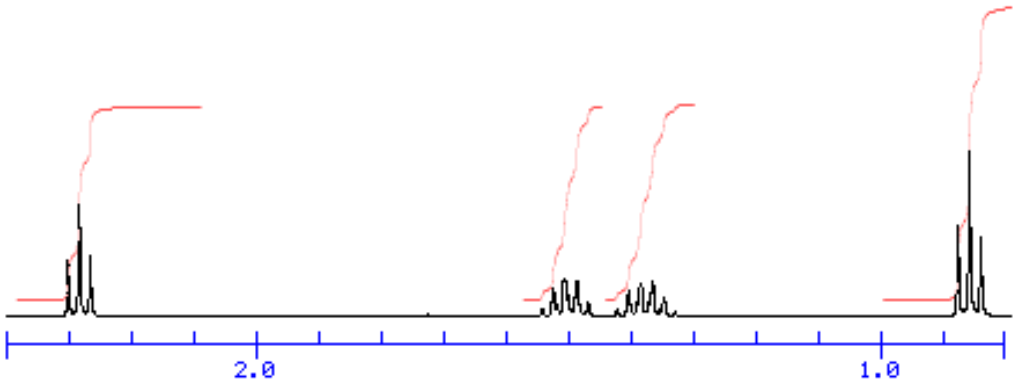
ANSWER

34- Spectra are shown for a molecule of formula **$C_8H_{12}O_2$.** Propose a structure (write final answer in the box).

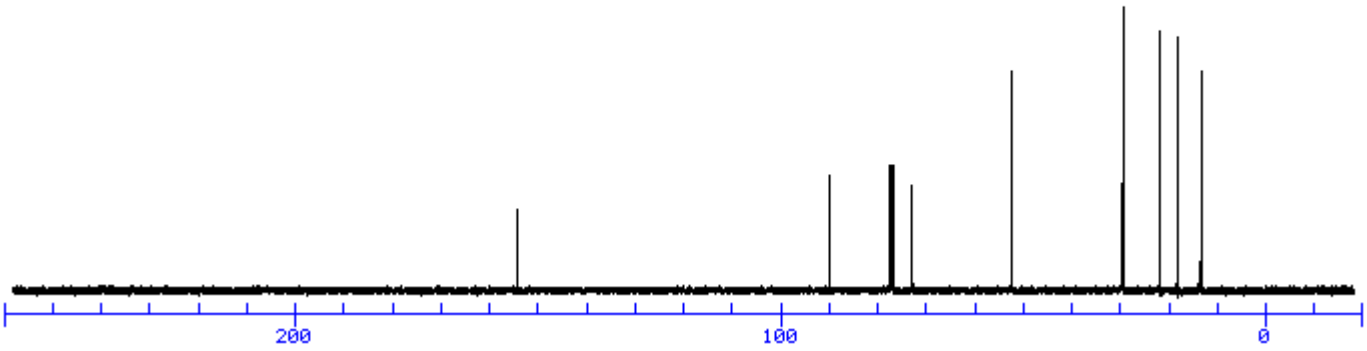
1H NMR (showing only the area with signals) **ANSWER**



1H NMR expansion

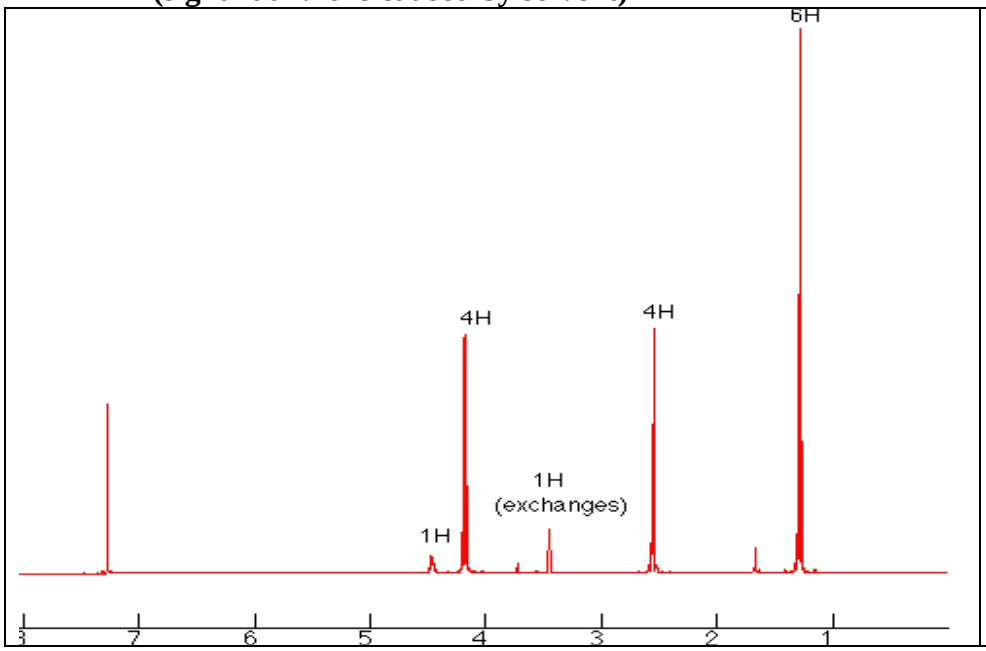


13C NMR (thick signal at ~77 ppm is due to solvent)



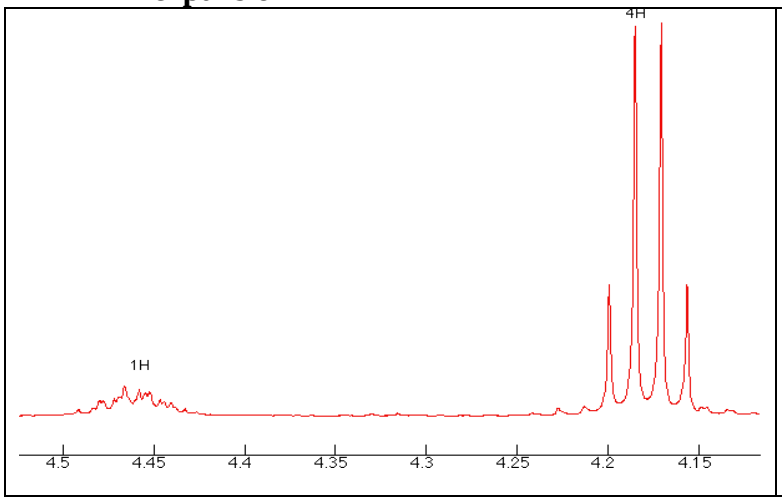
35- Spectra are shown for a molecule of formula **$C_9H_{16}O_5$.** Propose a structure (write final answer in the box).

1H NMR (signal at 7.26 is caused by solvent)

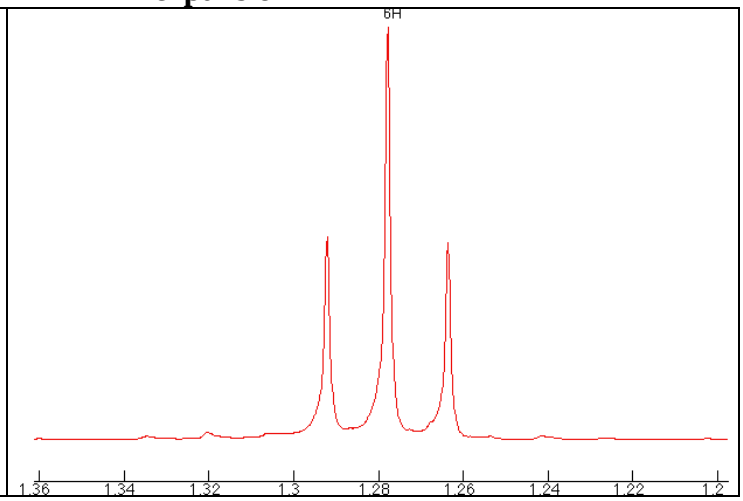


ANSWER

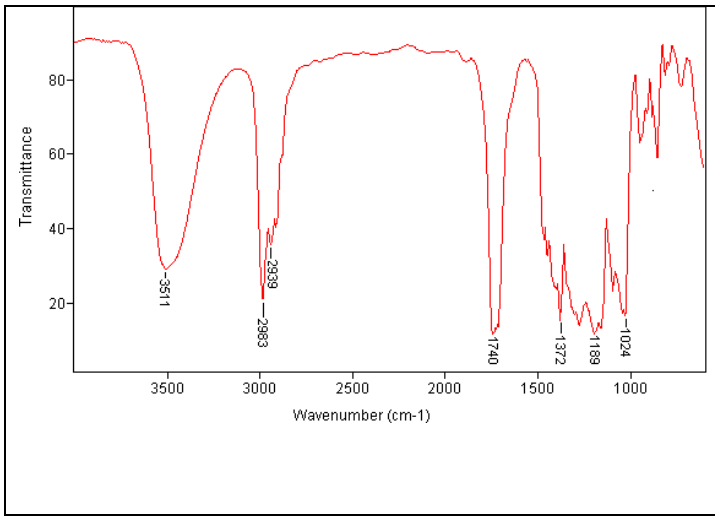
1H NMR expansion



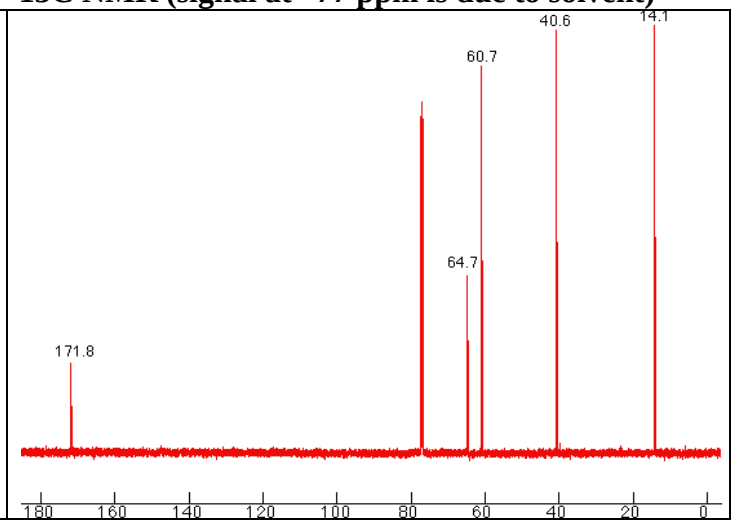
1H NMR expansion



IR

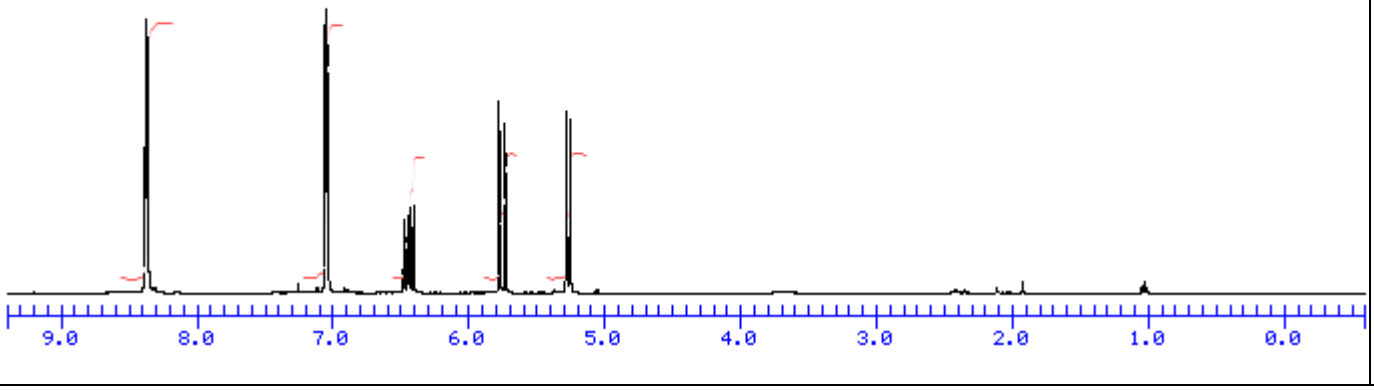


13C NMR (signal at ~77 ppm is due to solvent)

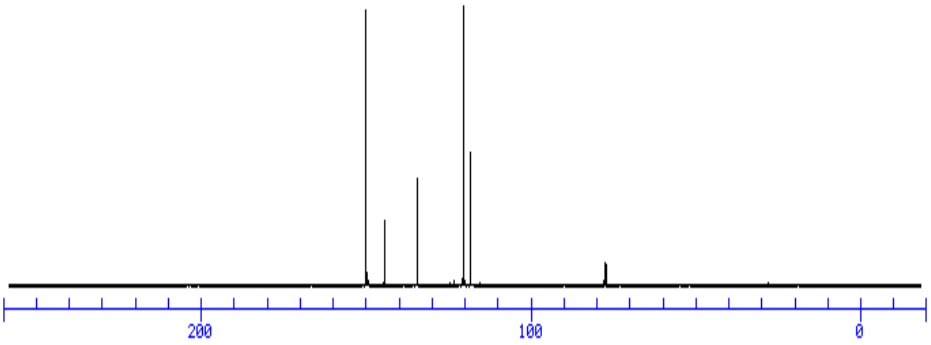


36- Spectra are shown for a molecule of formula **C_7H_7N.** Propose a structure (write final answer in the box).

1H NMR

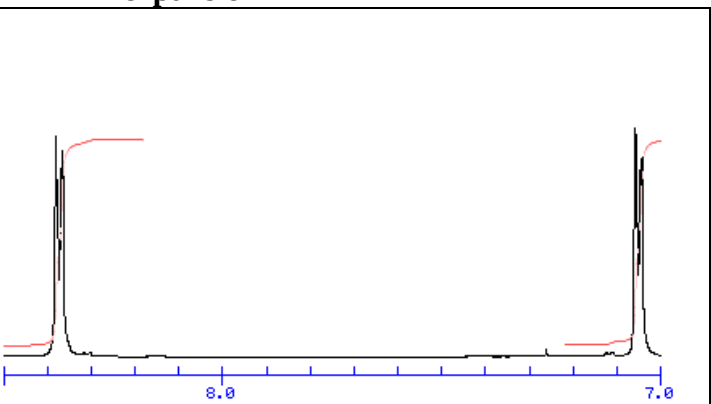


13C NMR (tiny signal at 77 ppm is due to solvent)

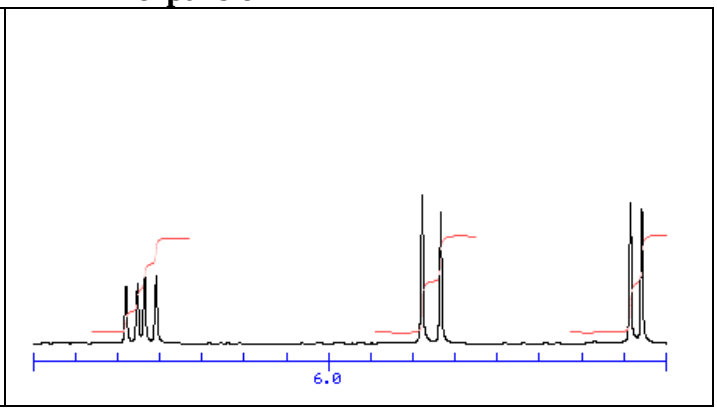


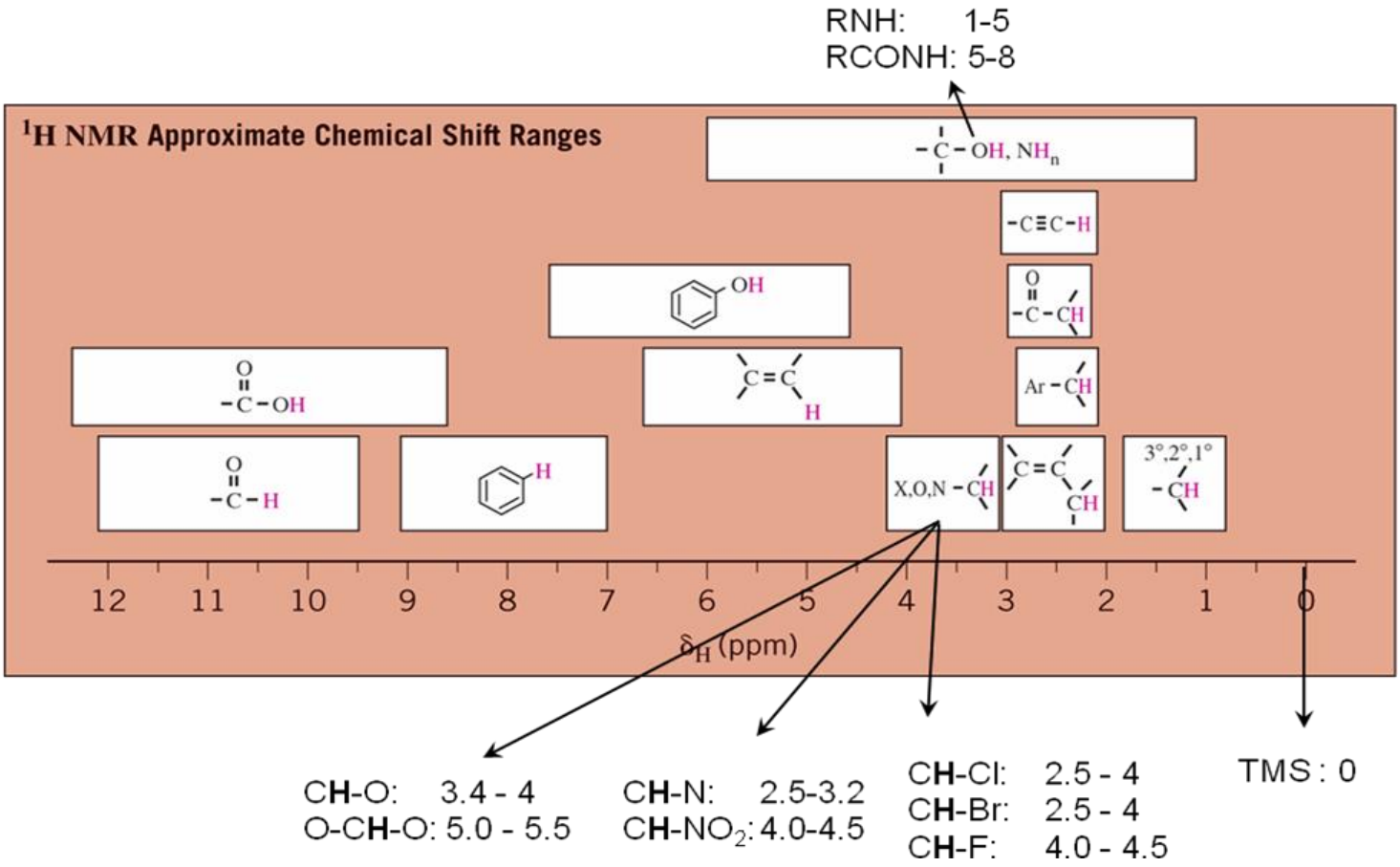
ANSWER

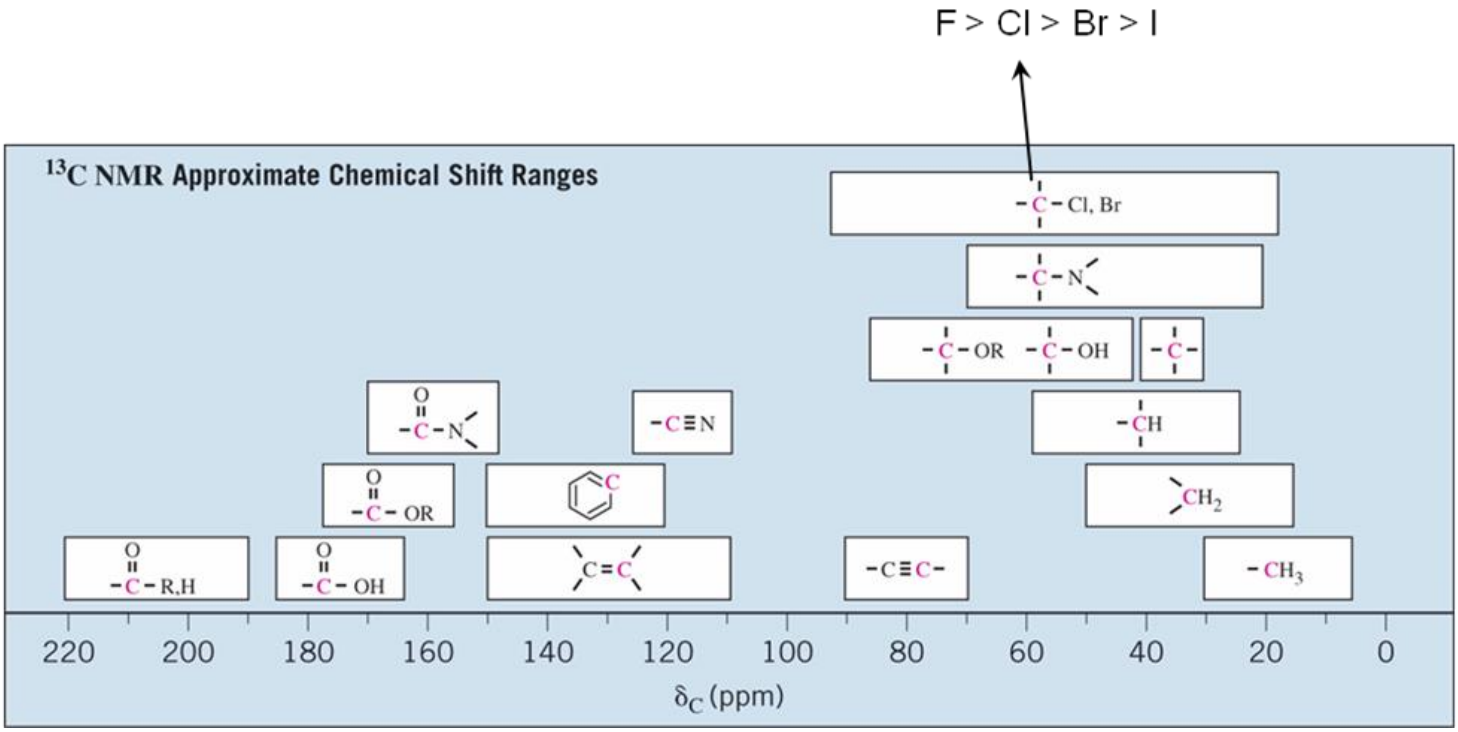
1H NMR expansion



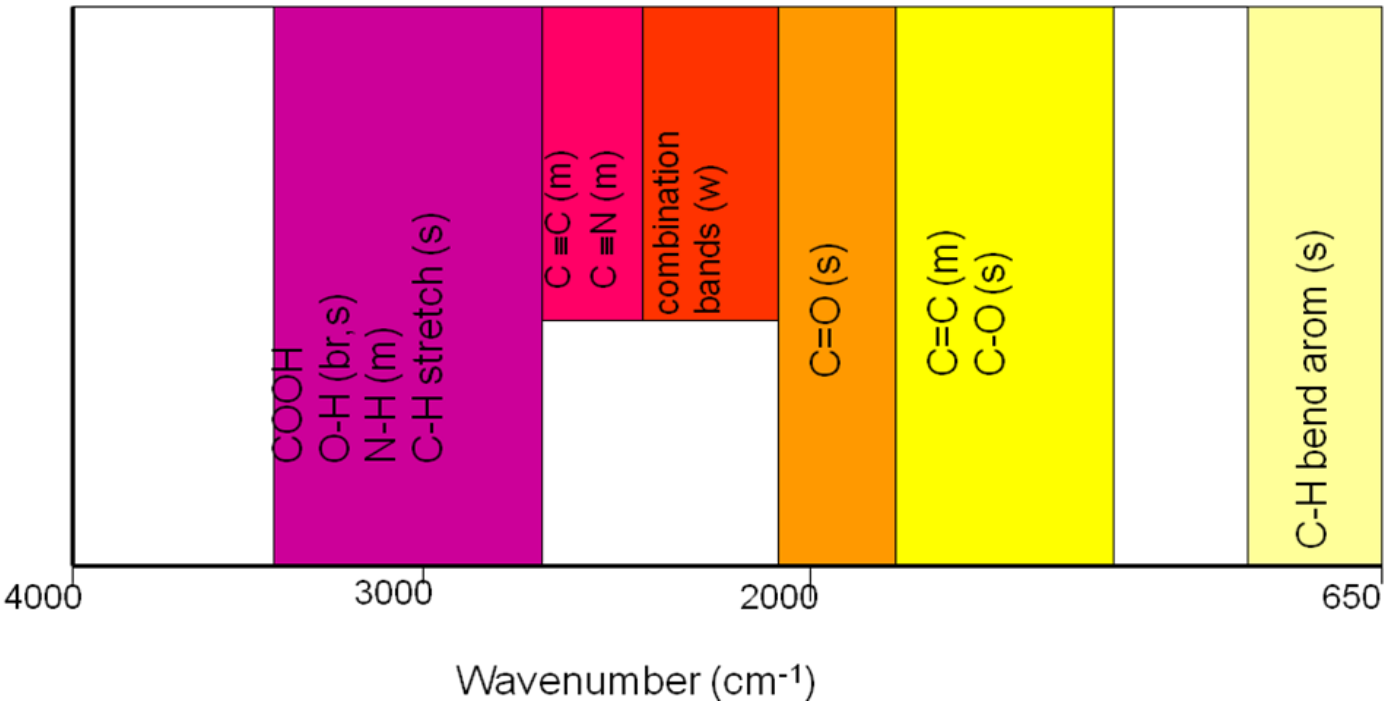
1H NMR expansion




RNH: 1-5
RCONH: 5-8
1H NMR Approximate Chemical Shift Ranges
-C-OH, NHn
-C≡C-H
OH
-C-CH
-C-OH
C=C
H
Ar-CH
-C-H
H
X,O,N-CH
C=C
CH
3°,2°,1°
-CH
12 11 10 9 8 7 6 5 4 3 2 1 0
δH (ppm)
CH-O: 3.4 - 4
O-CH-O: 5.0 - 5.5
CH-N: 2.5-3.2
CH-NO2: 4.0-4.5
CH-Cl: 2.5 - 4
CH-Br: 2.5 - 4
CH-F: 4.0 - 4.5
TMS : 0


F > Cl > Br > I
13C NMR Approximate Chemical Shift Ranges
-C-Cl, Br
-C-N
-C-OR
-C-OH
-C-
-C≡N
-CH
-C-OR
CH2
-C-R,H
-C-OH
C=C
-C≡C-
-CH3
220 200 180 160 140 120 100 80 60 40 20 0
δC (ppm)

IR Absorption Ranges



Group		Frequency Range (cm^{-1})	Intensity[a]
A. Alkyl			
C—H (stretching)		2853–2962	(m–s)
Isopropyl, $—CH(CH_3)_2$		1380–1385	(s)
	and	1365–1370	(s)
tert-Butyl, $—C(CH_3)_3$		1385–1395	(m)
	and	~1365	(s)
B. Alkenyl			
C—H (stretching)		3010–3095	(m)
C=C (stretching)		1620–1680	(v)
R—CH=CH_2	(out-of-plane C—H bendings)	985–1000	(s)
	and	905–920	(s)
$R_2C=CH_2$		880–900	(s)
cis-RCH=CHR		675–730	(s)
trans-RCH=CHR		960–975	(s)
C. Alkynyl			
≡C—H (stretching)		~3300	(s)
C≡C (stretching)		2100–2260	(v)
D. Aromatic			
Ar—H (stretching)		~3030	(v)
Aromatic substitution type (C—H out-of-plane bendings)			
Monosubstituted		690–710	(very s)
o-Disubstituted	and	730–770	(very s)
m-Disubstituted		735–770	(s)
		680–725	(s)
	and	750–810	(very s)
p-Disubstituted		800–860	(very s)
E. Alcohols, Phenols, and Carboxylic Acids			
O—H (stretching)			
Alcohols, phenols (dilute solutions)		3590–3650	(sharp, v)
Alcohols, phenols (hydrogen bonded)		3200–3550	(broad, s)
Carboxylic acids (hydrogen bonded)		2500–3000	(broad, v)
F. Aldehydes, Ketones, Esters, and Carboxylic Acids			
C=O (stretching)		1630–1780	(s)
Aldehydes		1690–1740	(s)
Ketones		1680–1750	(s)
Esters		1735–1750	(s)
Carboxylic acids		1710–1780	(s)
Amides		1630–1690	(s)
G. Amines			
N—H		3300–3500	(m)
H. Nitriles			
C≡N		2220–2260	(m)

[a]Abbreviations: s = strong, m = medium, w = weak, v = variable, ~ = approximately.

SCRAP PAGE

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