Spectroscopies Worksheet

Name Answer Key

This is an exercise to give you more experience with interpretation of spectral data.

- It is a 50 point exercise that I am asking you to turn in at or before class on Thursday, Feb. 26.
- You may (in fact, you should) work together, but each of you must turn in your own set of final answers.
- This exercise is meant to be a learning tool so that all of you can improve your ability to interpret spectral data. Use notes, the internet, and each other as resources. I will not tell you the answers, but I will answer specific and thoughtful questions, though, provided you have put some effort into the issue at hand.
- You will learn things from this exercise that will enhance your ability to interpret spectral data and identify compounds.

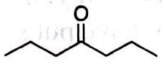
Part I.

The three mass spectra (**A-C**) for this problem are located on page 4. The three compounds giving rise to these spectra are *among* the five shown below (**1-5**). Give the structure of the ion responsible for each of the peaks labeled with the number of its mass on each of the mass spectra (draw your structures directly on each mass spectrum).

- Label the structure responsible for spectrum **A** with "**A**"
- Label the structure responsible for spectrum **B** with "**B**"
- Label the structure responsible for spectrum **C** with "**C**"

(Leave the remaining two structures blank)

4-heptanone



$C_7H_{14}O$

1

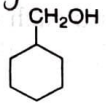
octane

C_8H_{18}

2

C

cyclohexylmethanol

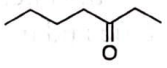


$C_7H_{14}O$

3

A

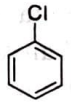
3-heptanone



$C_7H_{14}O$

4

chlorobenzene



C_6H_5Cl

5

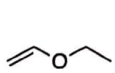
B

Part II.

The three infrared spectra (**D-F**) for this problem are located on page 5. The three compounds giving rise to these spectra are *among* the six shown below (**7-12**).

- Label the structure responsible for spectrum **D** with "**D**"
- Label the structure responsible for spectrum **E** with "**E**"
- Label the structure responsible for spectrum **F** with "**F**"

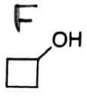
(Leave the remaining three structures blank)



7

ethoxyethene

F



8

cyclobutanol

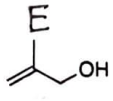
9

oxolane
tetrahydrofuran

10

2-butanone

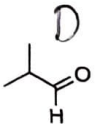
E



11

2-methyl-2-propen-1-ol

D



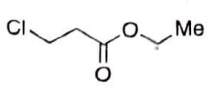
12

2-methyl-1-propanal

Part III.

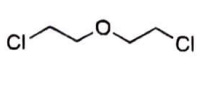
The three proton NMR spectra (**G-I**) for this problem are located on page 6. The three compounds giving rise to these spectra are *among* the six shown below (**13-18**). I have labeled each resonance with the *relative* intensity of the peaks (i.e., the integral) and, where necessary for clarity, the multiplicity.

- Label the structure responsible for spectrum **G** with "**G**"
- Label the structure responsible for spectrum **H** with "**H**"
- Label the structure responsible for spectrum **I** with "**I**"
- (Leave the remaining three structures blank)

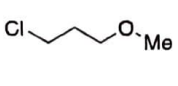


13

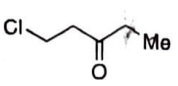
G



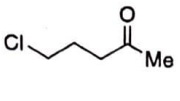
14



15

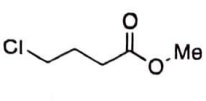


16



17

H



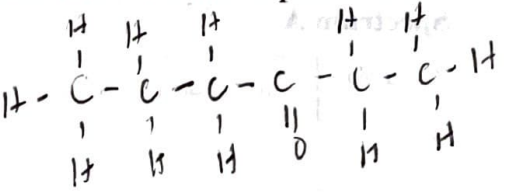
18

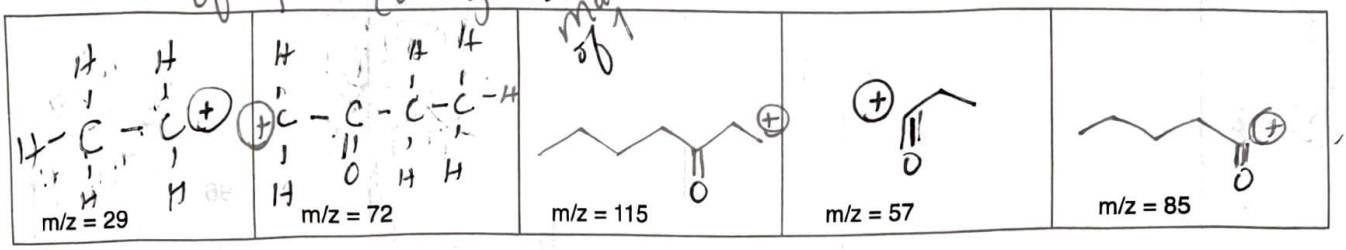
I

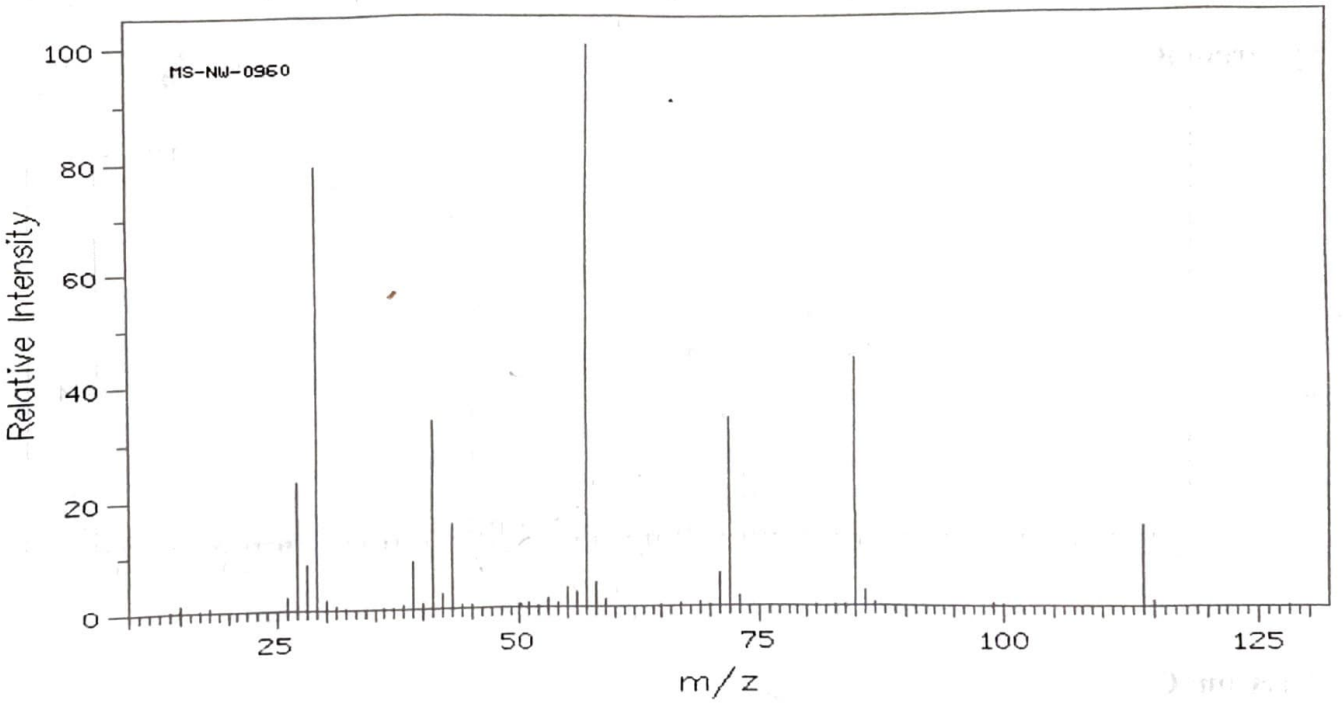
Part IV

The mass spectrum below is that of 3-heptanone (**19**). Indicate the structure of the ion responsible for the peak at each of the following five masses (*m/z*).

Note: 3-heptanone often gets protonated @ the carbonyl group to add a mass of 1

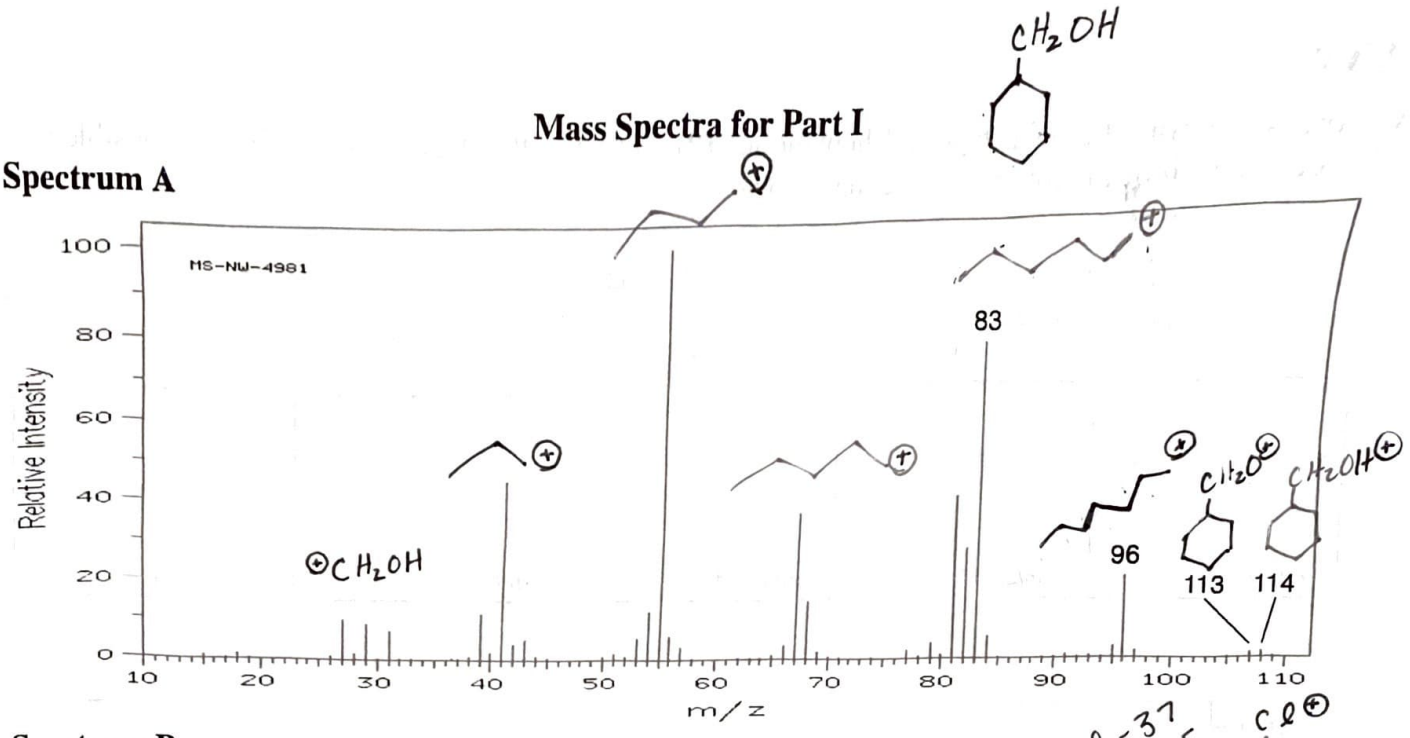




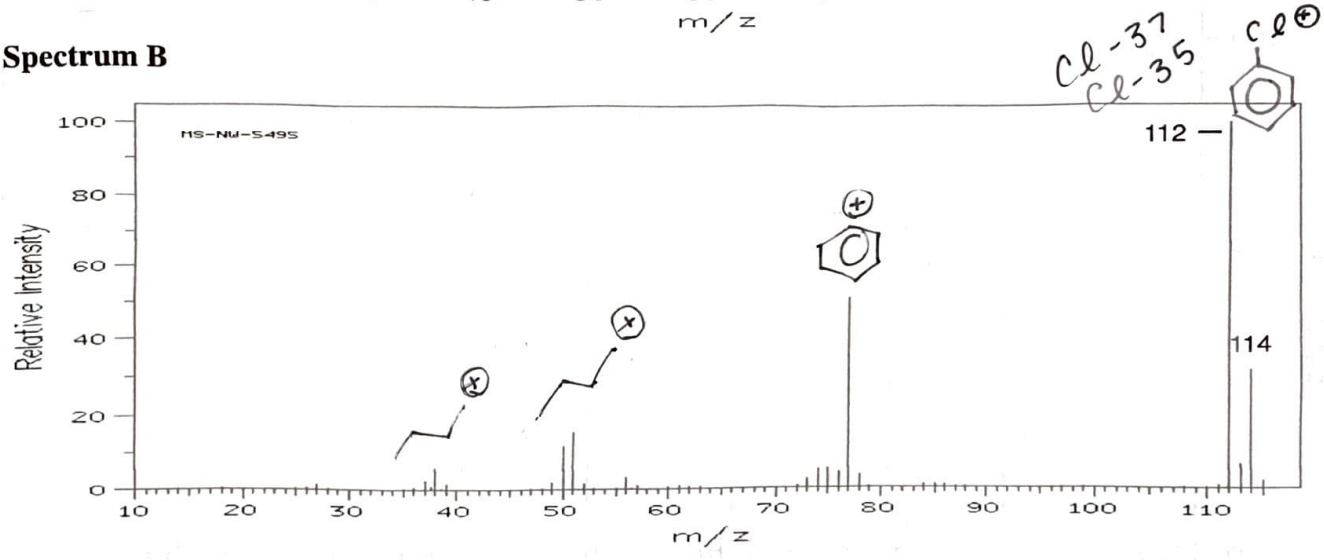


Mass Spectra for Part I

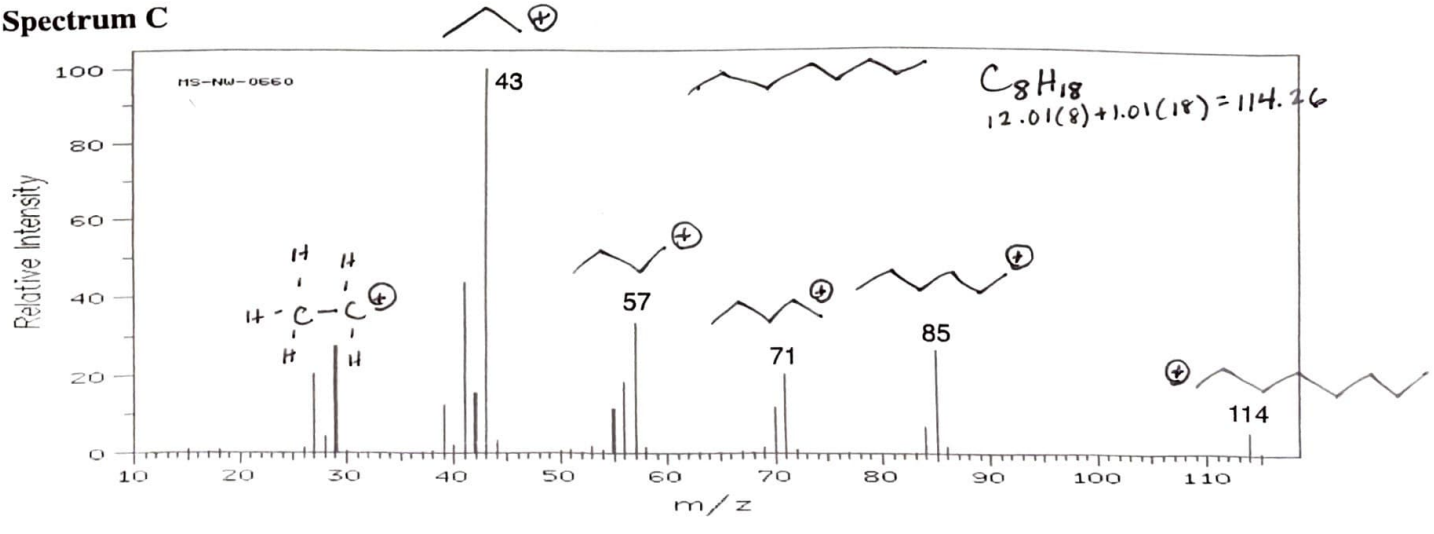
Spectrum A



Spectrum B

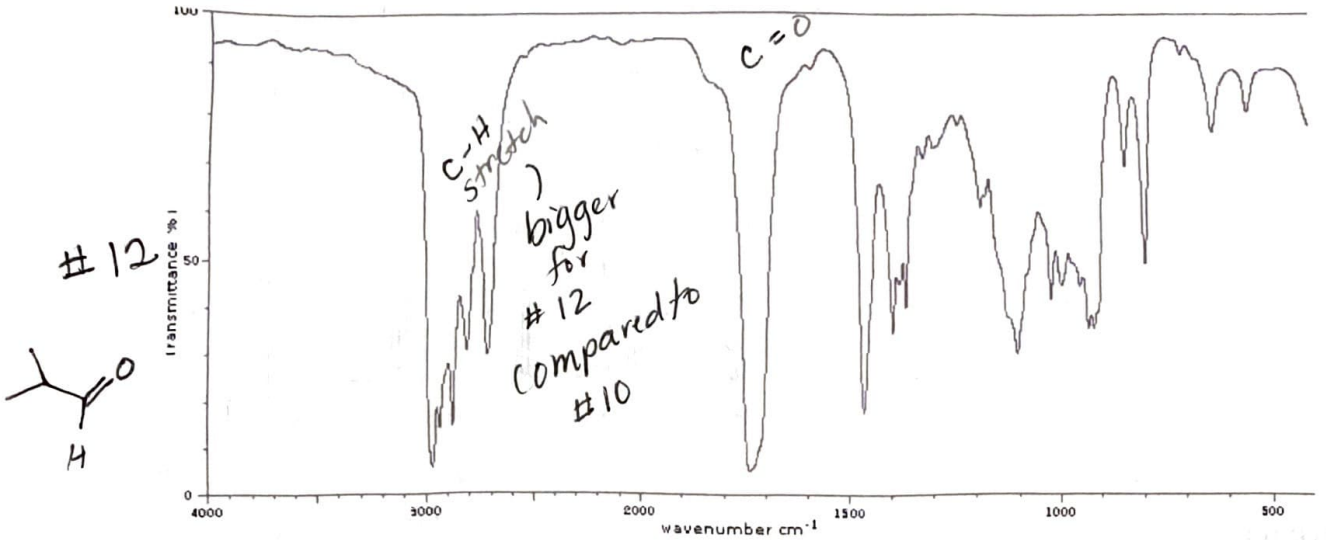


Spectrum C

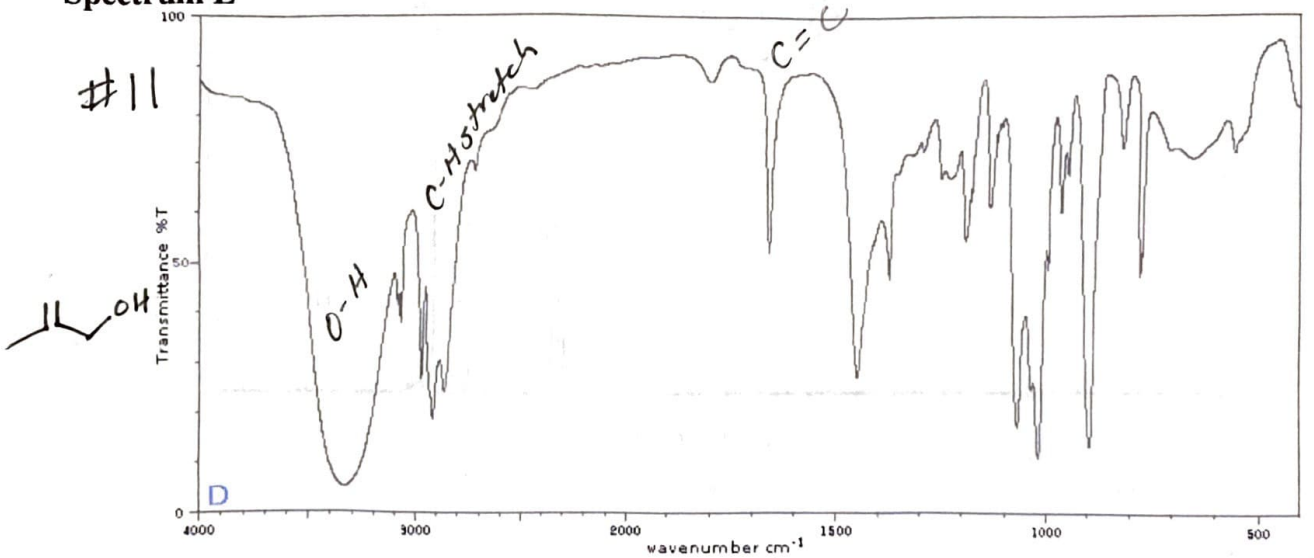


Infrared Spectra for Part II

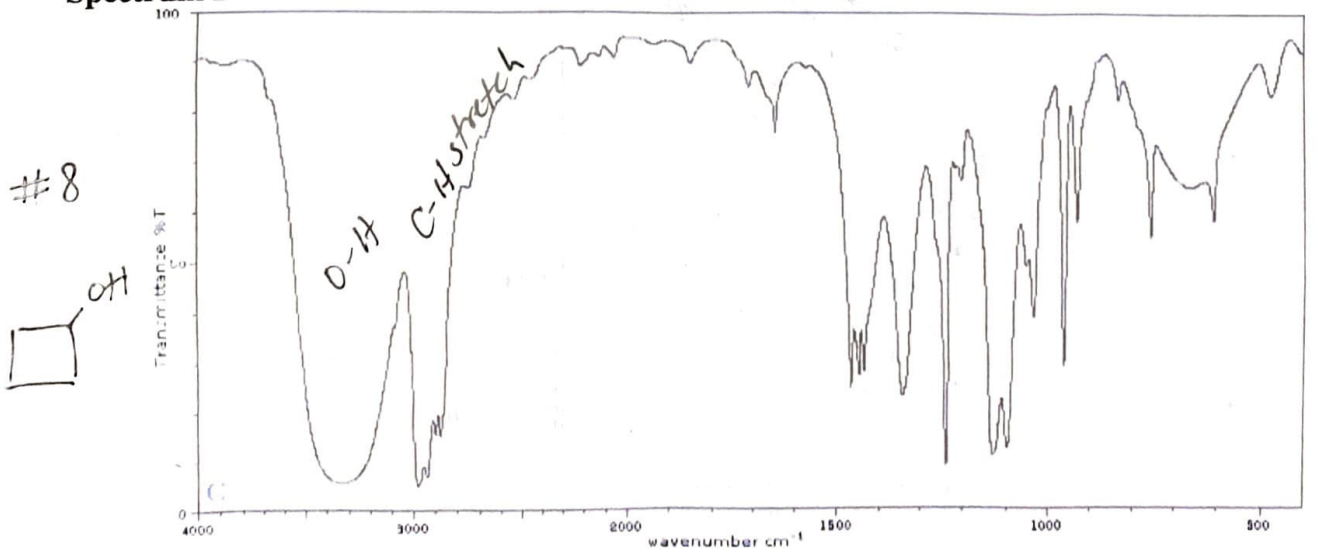
Spectrum D



Spectrum E

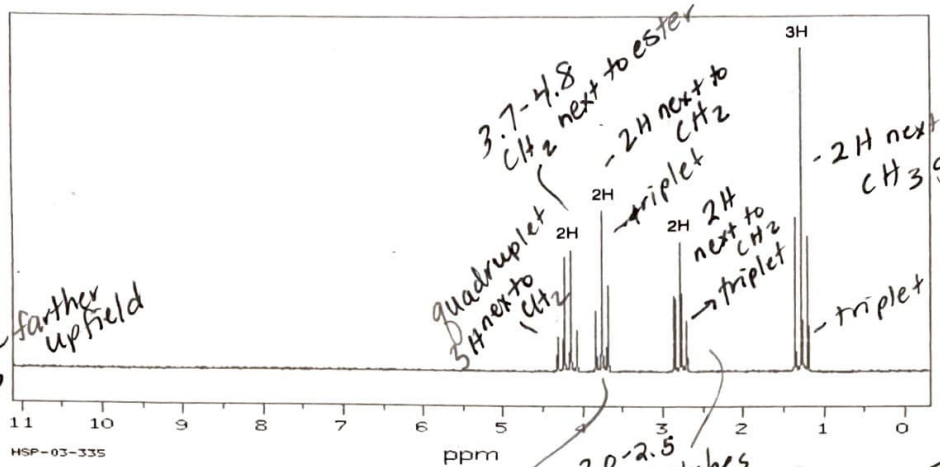


Spectrum F



Proton NMR Spectra for Part III

Spectrum G



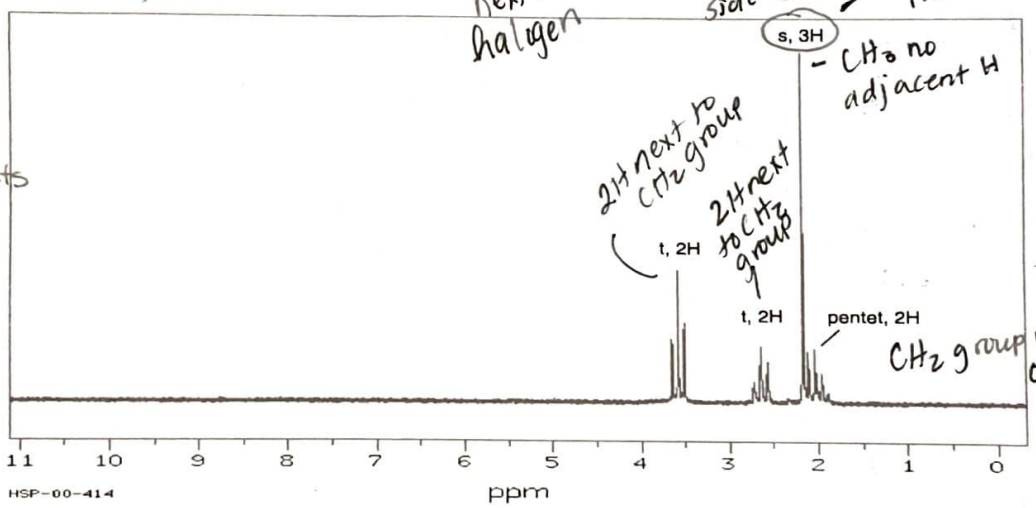
4H environments

options: (13) 15 singlet 16 - ketone 17 singlets farther upfield

next to halogen

2.0-2.5 matches CH_2 on other side of ester

Spectrum H



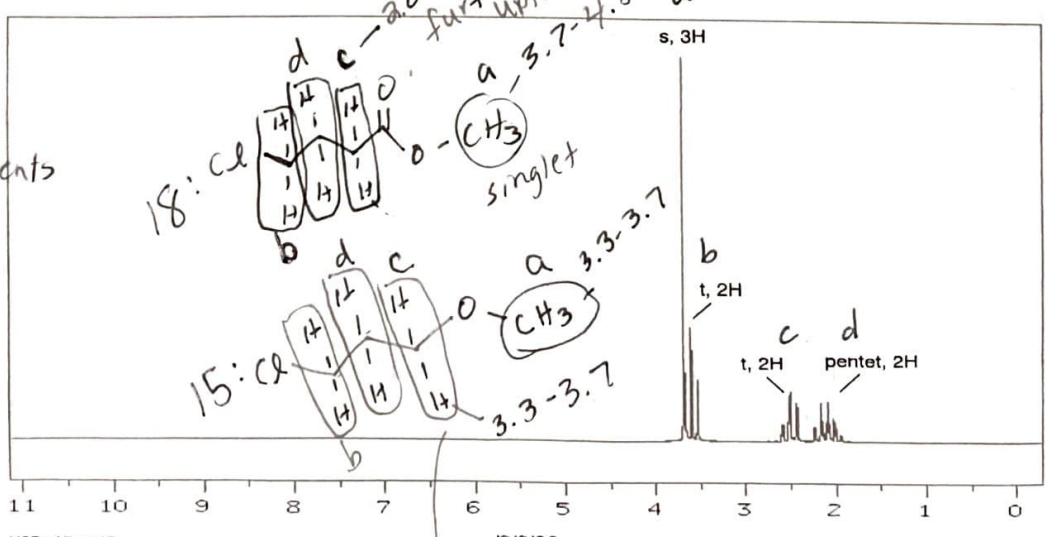
4H environments w/singlet

options

~~16~~ O-me

(17) C-me

Spectrum I



4 H environments

options

(16) 15

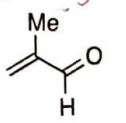
6 should be farther downfield

Part V.

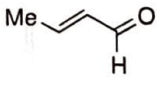
On the following three pages (pp 8-10) are eight nmr, ir, and/or mass spectra labeled **Spectrum 1** through **Spectrum 8**. Each is of one of the sixteen structures listed below (**A-P**). All of these possible answers have the same molecular formula (i.e., C_4H_6O). All of your answers for this problem should appear in the boxes on the bottom of this page.

Assign the correct structure to each **Spectrum #** by adding the appropriate letter to the box beside each **Spectrum #** at the bottom of this page. Note: it is possible that the same structure (i.e., letter) could be the correct answer for more than one **Spectrum #**.

methacrylaldehyde

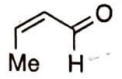


A C_4H_6O



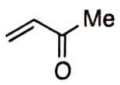
B

cis 2-butenal



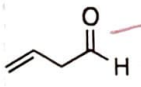
C C_4H_6O

3-buten-2-one



D C_4H_6O

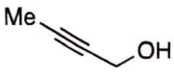
3-butenal



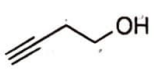
more intense C=O due to closer C=C bond

E C_4H_6O

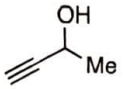
F



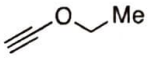
G



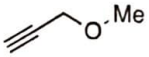
H



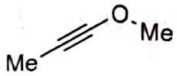
I



J



K



L

M

N

O

P

Spectrum 1 B

Spectrum 2 M

Spectrum 3 F

Spectrum 4 I

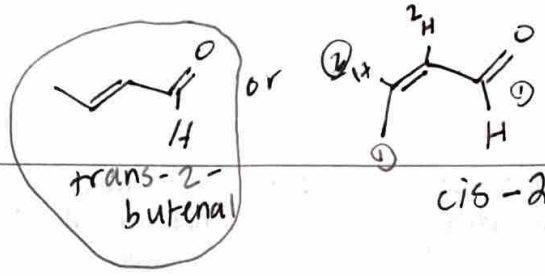
Spectrum 5 H

Spectrum 6 M

Spectrum 7 O

Spectrum 8 I

Spectrum 1



trans-2-butenal

or

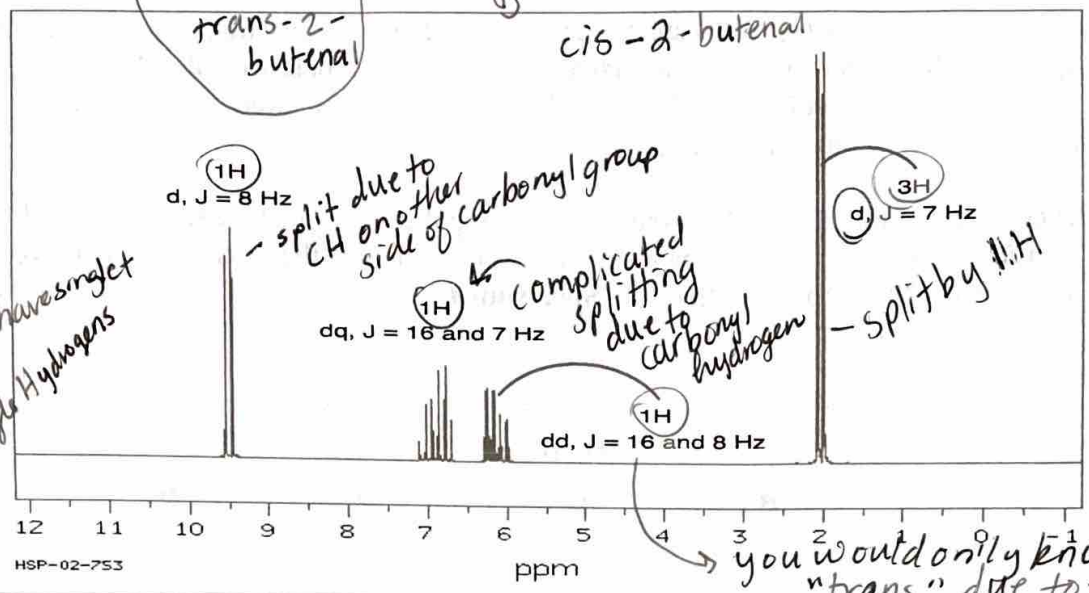
cis-2-butenal

4 unique H environments possibilities:

B
C

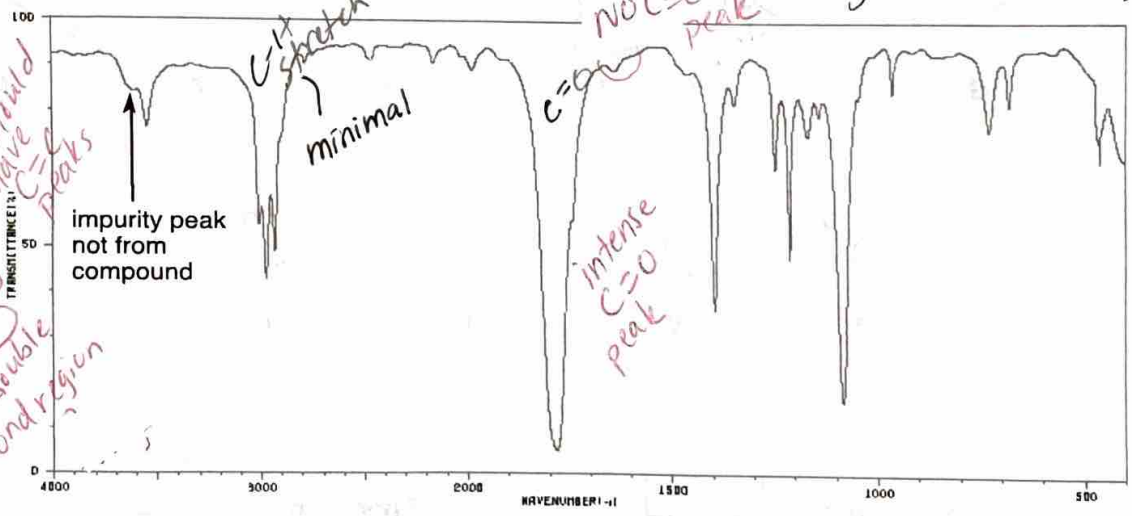
~~A~~ - would have singlet

~~D~~ ~~E~~ ~~F~~ ~~G~~ not 3 single Hydrogens



you would only know this was "trans" due to these higher J values (you don't have to know this)

Spectrum 2

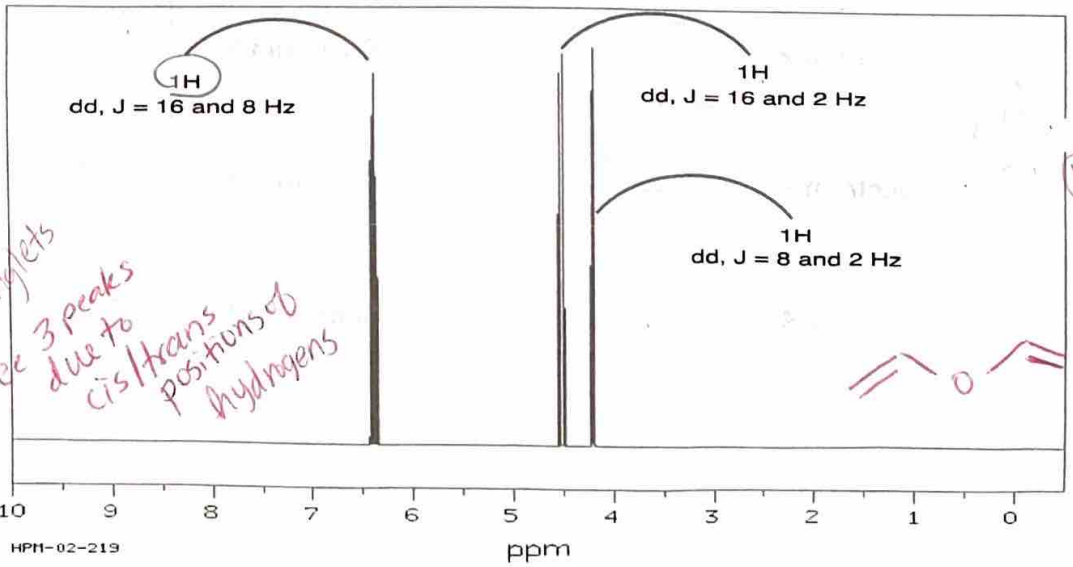


options:

~~A~~ ~~C~~ ~~D~~ ~~E~~ all should have C=C peaks

M no C=C double bond region

Spectrum 3

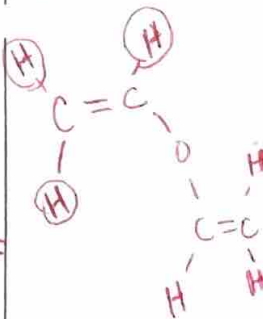


3 unique H environments:

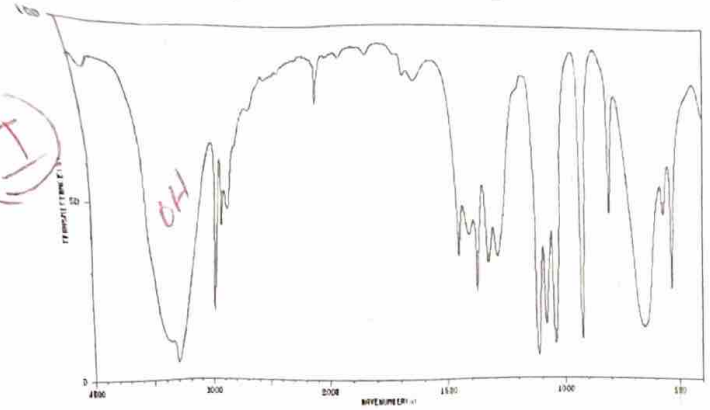
options

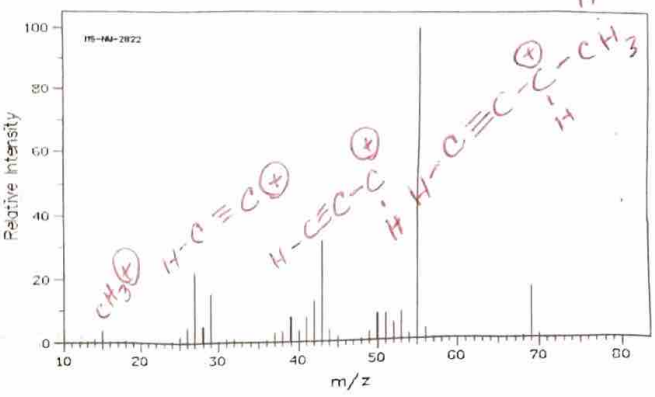
~~A~~ ~~D~~ nonsinglets

F see 3 peaks due to cis/trans positions of hydrogens

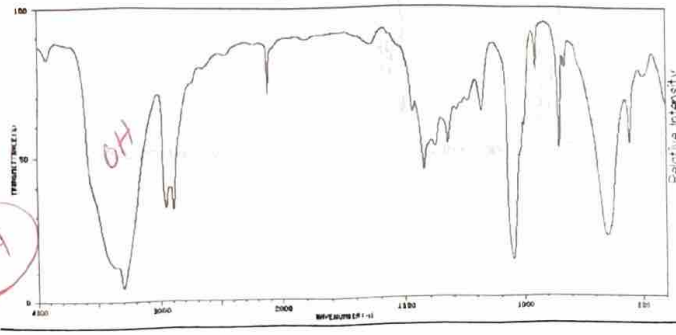


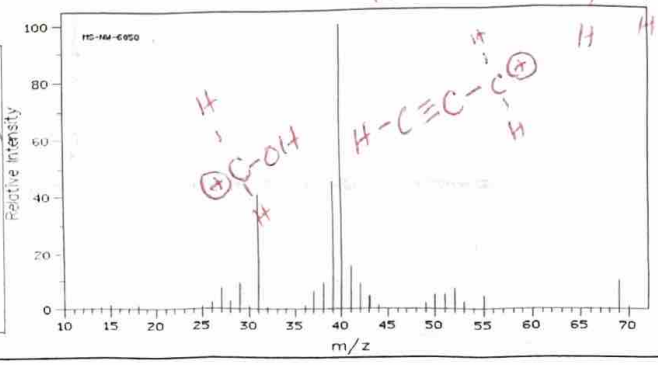
Spectrum 4 (these IR and mass spectra are both of the same compound) 3-butyn-2-ol



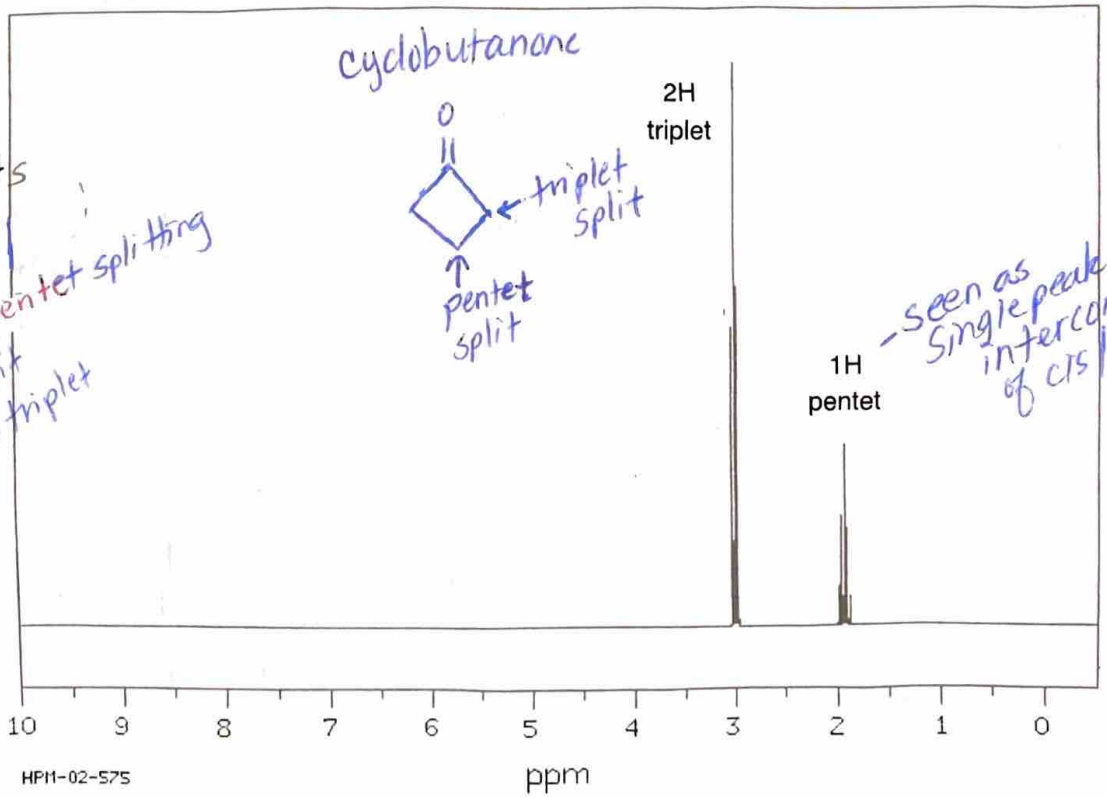


Spectrum 5 (these IR and mass spectra are both of the same compound) 3-butyn-1-ol





Spectrum 6



cyclobutanone

triplet split

pentet split

2 unique H environments

options:

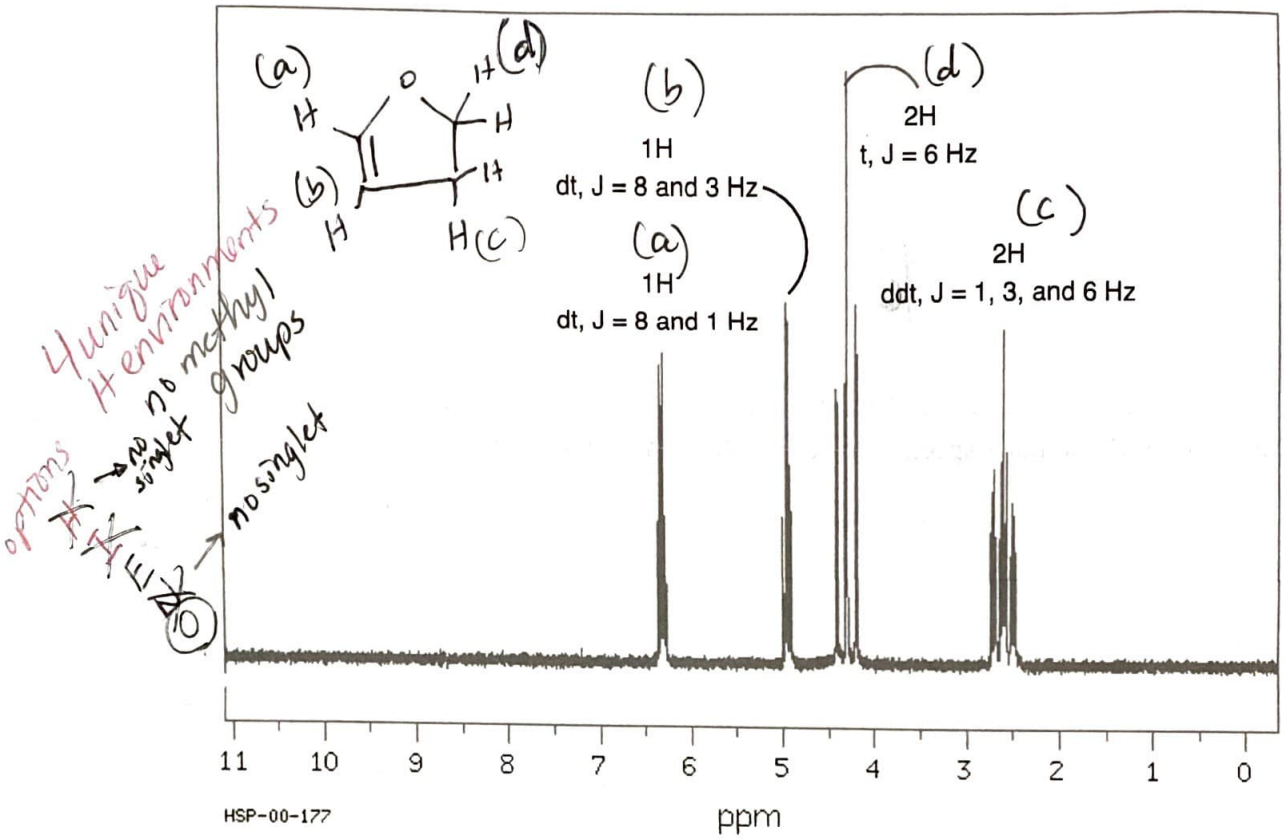
M

X - no pentet splitting

X - 1H split into triplet

- seen as single peak due to interconversion of cis/trans isomers

Spectrum 7



Spectrum 8