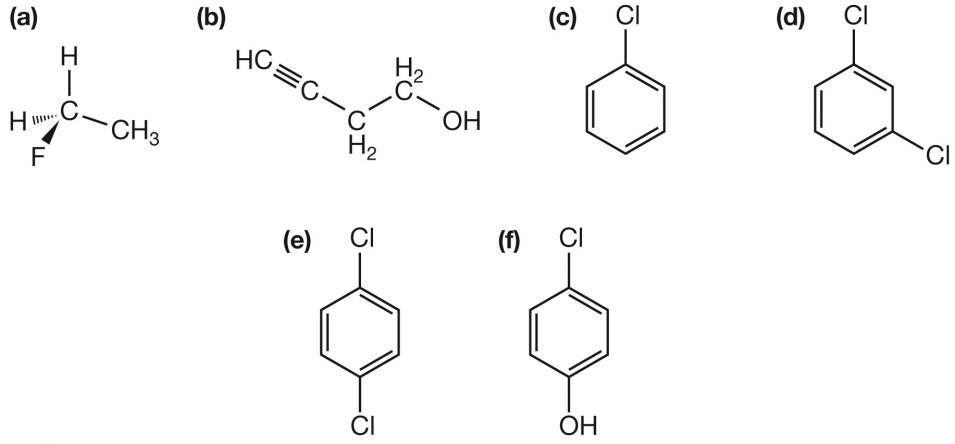
Chapter 17 Homework – Nuclear Magnetic Resonance (NMR)

Part A. Carbon Nuclear Magnetic Resonance, ^{13}C NMR

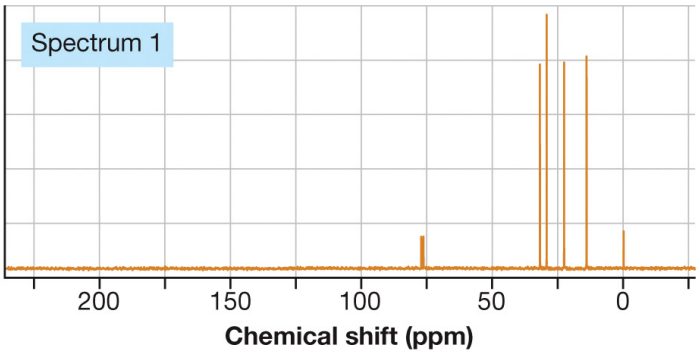
1. **How many signals** are expected in each compound's ^{13}C NMR spectrum?

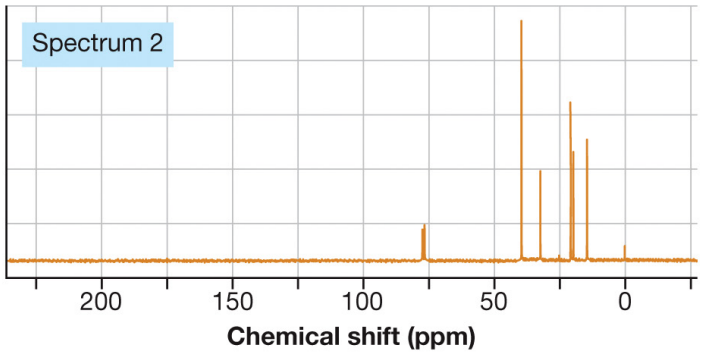


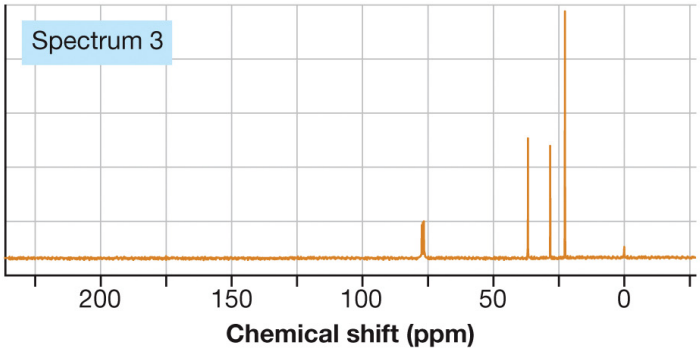
	Number of ^{13}C NMR signals
(a)	
(b)	
(c)	
(d)	
(e)	
(f)	

2. The ^{13}C NMR spectra of three isomers with molecular formula C_8H_{18} are given below. **Match each chemical name to its spectrum (1-3)**. Ignore the peak at 76 ppm (solvent).

Isomer	**Spectrum (1, 2, or 3?)**
2,5-dimethylhexane	
4-methylheptane	
Octane	

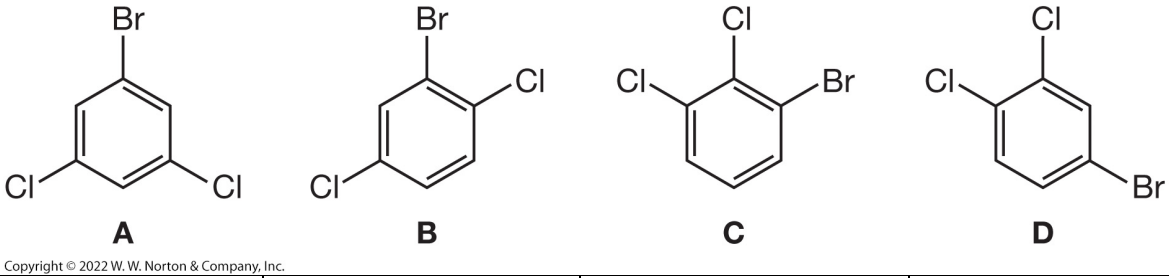






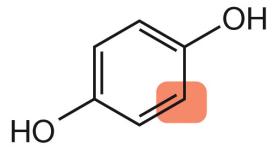
Ch 17A. ^{13}C NMR

3. **How many signals** are expected in each compound's ^{13}C NMR spectrum?



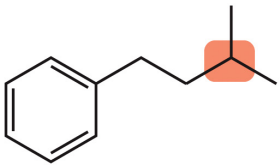
4. Indicate the **approximate chemical shift (range)** of each highlighted carbon in its ^{13}C NMR spectrum (Table 17-5).

(a)



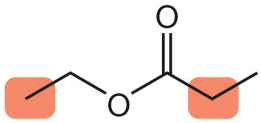
CH

(b)



CH

(c)

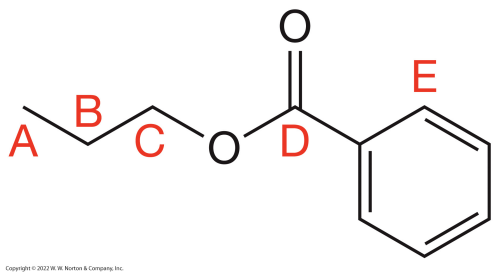


CH_3

20-35

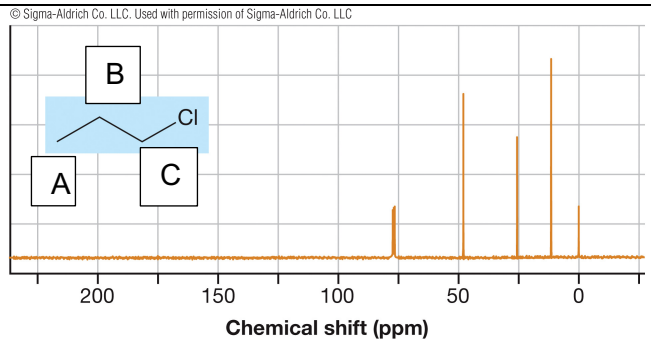
CH_2

5. **Indicate the expected ^{13}C NMR chemical shift range** for each carbon (A-E) in the table below.



Signal	Chemical shift range (ppm) Table 17-5
A	
B	
C	
D	
E	

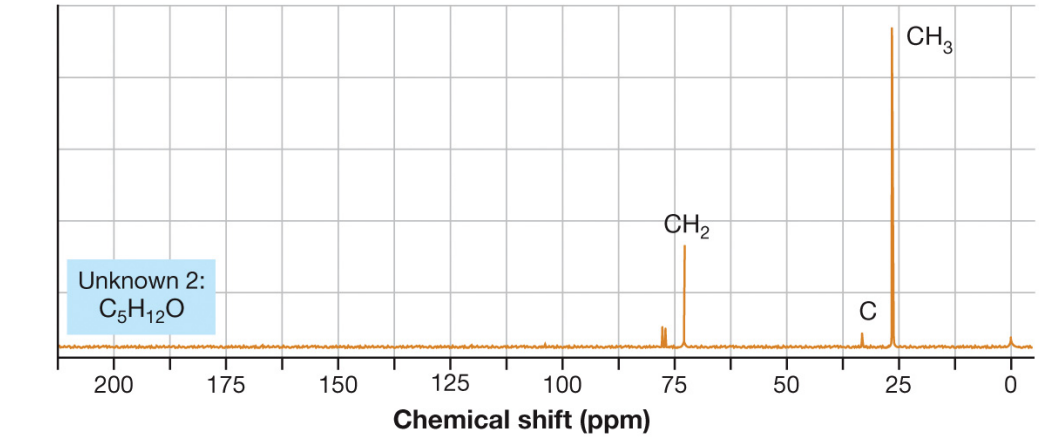
6. 1-chloropropane produced the ^{13}C NMR spectrum shown here. **Match each carbon** in the molecule (letters A-C) to each signal in the spectrum.

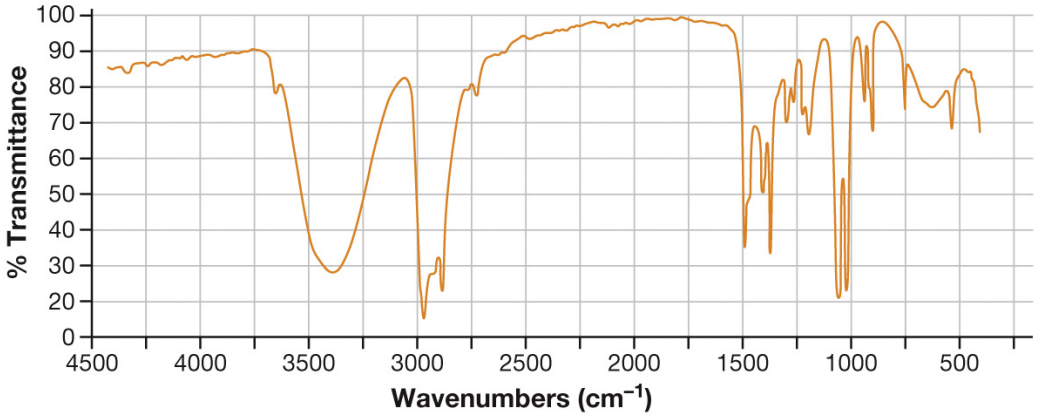


Signal (ppm)	Carbon (A, B, or C)
10	
25	
49	

Ch 17, Part A. ^{13}C NMR

7. **Propose the structure** of the molecule that matches the spectral data below.





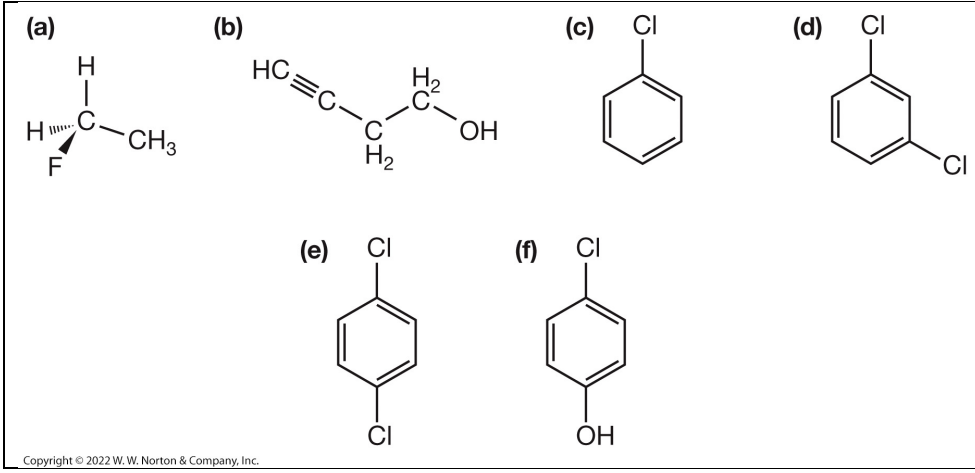
What clues does the **^{13}C NMR** spectrum provide about the structure?

What clues does the **IR spectrum** provide about the structure?

Structure:

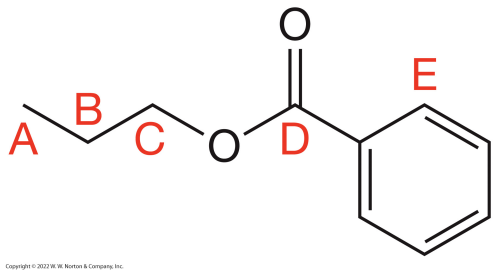
Chapter 17 HW, Part B. Proton Nuclear Magnetic Resonance, ^{1}H NMR

8. **How many signals** are expected in each compound's ^{1}H NMR spectrum?



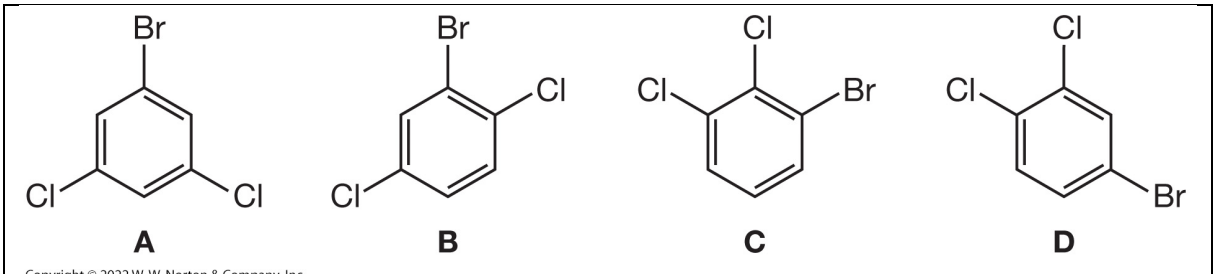
	Number of ^{1}H NMR signals
(a)	
(b)	
(c)	
(d)	
(e)	
(f)	

9. Indicate the **approximate ^{1}H NMR chemical shift** for each carbon (A-E) in the table below.



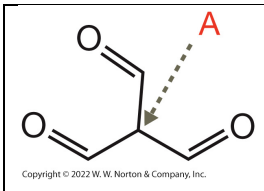
Signal	Chemical shift (ppm) Table 17-1
A	
B	
C	
D	
E	

10. **How many signals** are expected in each compound's ^{1}H NMR spectrum?



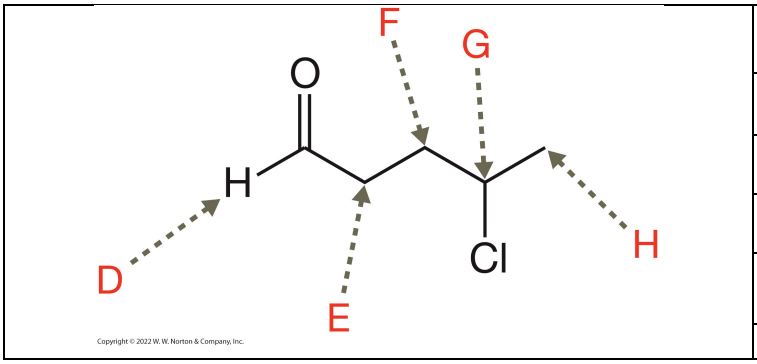
Chapter 17B. ^{1}H NMR

11. Rank protons A-C in order from **largest to smallest chemical shift.** Write the proton's letter in the right column of the table. Then, provide the **integration value** (number of H's) responsible for each signal.



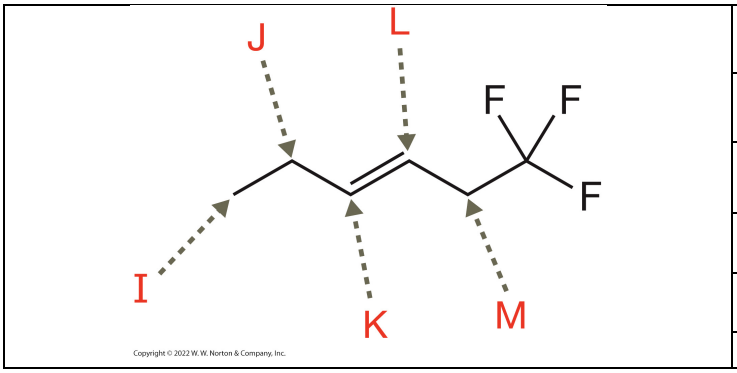
Chemical Shift Rank	Proton (A-C)	Integration (# of H's)
High		
Medium		
Low		

12. Rank protons D-H in order from **largest to smallest chemical shift.** Write the proton's letter in the right column of the table.



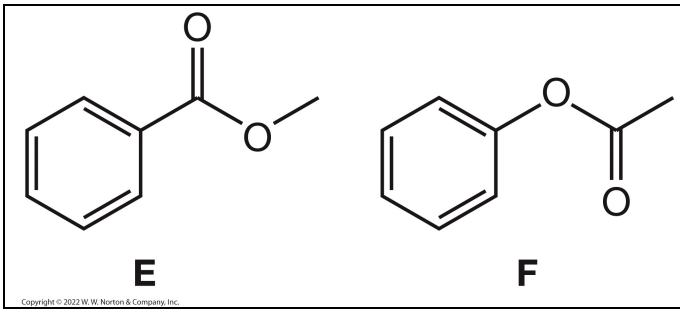
Chemical Shift Rank	Proton (D-H)	Integration (# of H's)
Highest		
Lowest		

13. Rank protons I-M in order from **largest chemical shift to smallest.** Write the proton's letter in the right column of the table.



Chemical Shift Rank	Proton (I-M)	Integration (# of H's)
Highest		
Lowest		

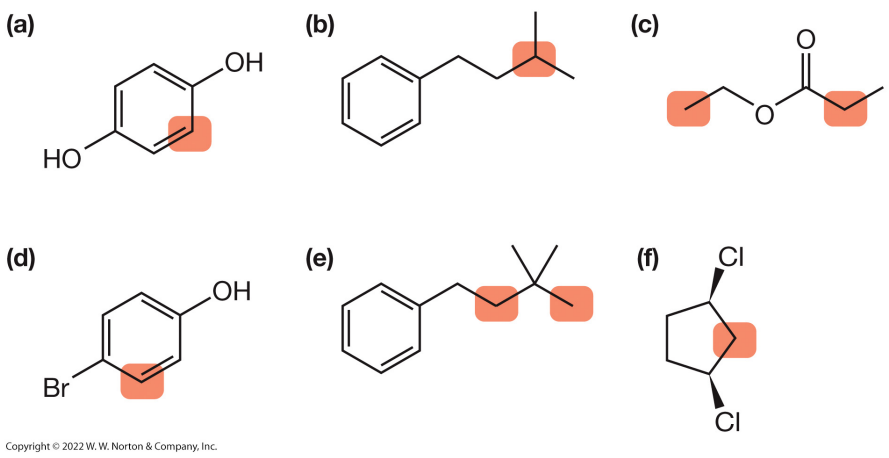
14. Report the approximate **^{1}H NMR** and **^{13}C NMR chemical shifts of just the <u>CH_3 group</u>** in similar benzylic esters **E** and **F** below.



	^{1}H NMR (Table 17-1)	^{13}C NMR (Table 17-5)
E		
F		

Chapter 17B. ^{1}H NMR

15. Use the N+1 rule, where N is the number of adjacent H's, to predict **splitting pattern** of the highlighted signal in its ^{1}H NMR spectrum (singlet, doublet, triplet, quartet, pentet, sextet, septet, octet, or nonet).



	Splitting Pattern(s)
(a)	
(b)	
(c)	CH_3 group: CH_2 group:
(d)	
(e)	CH_2 group: CH_3 group:
(f)	

16. **<u>Structural Elucidation</u>**: use the data below to determine the structure of the compound.

		What does each piece of data tell you about the compound?
Formula	C_3H_6O	Any double bonds?
IR	1720 cm^{-1} (broad, strong) 2900 cm^{-1} (sharp, strong)	
^{1}H NMR	One signal… Chemical shift = 2.0 ppm Integration = 6H Splitting = singlet	
^{13}C NMR	δ 207 ppm δ 31 ppm	

Structure:

Chapter 17 HW

17. Structural Elucidation: use the data below to determine the structure of the compound.

<table>
<tr><td>Formula</td><td colspan="3">$C_5H_{12}O$</td><td>What does each signal tell you about the compound?
(show your work in the space below)</td></tr>
<tr><td>IR</td><td colspan="3">3300 cm^{-1}

2900 cm^{-1}</td><td></td></tr>
<tr><td>^{1}H NMR</td><td>Chemical shift</td><td>Integration (# of Hs)</td><td>Splitting</td><td rowspan="6"></td></tr>
<tr><td rowspan="5"></td><td>4.0 ppm</td><td>1</td><td>Broad singlet</td></tr>
<tr><td>3.5 ppm</td><td>2</td><td>Triplet</td></tr>
<tr><td>1.6 ppm</td><td>1</td><td>nonet</td></tr>
<tr><td>1.5 ppm</td><td>2</td><td>quartet</td></tr>
<tr><td>0.9 ppm</td><td>6</td><td>doublet</td></tr>
<tr><td>^{13}C NMR</td><td colspan="3">δ 61 (CH_2)

δ 42 (CH_2)

δ 25 (CH)

δ 23 (CH_3)</td><td></td></tr>
</table>

Structure:

This graded HW set includes problems adapted from the Karty 3 text.

Recommended Problems from Karty 3, Chapter 17 – see Canvas textbook module

- **In-Chapter Problems,** “Your Turn” = 1-4,7,8, 14-16, 20, 21, 24-27, 30
- **End-o-Chapter Problems** = 1-2, 6-9, 11, 12, 21, 24, 25, 29-35, 41, 44, 47, 49, 52, 53
  - Solutions to all problems are now available for FREE in the Canvas textbook module!