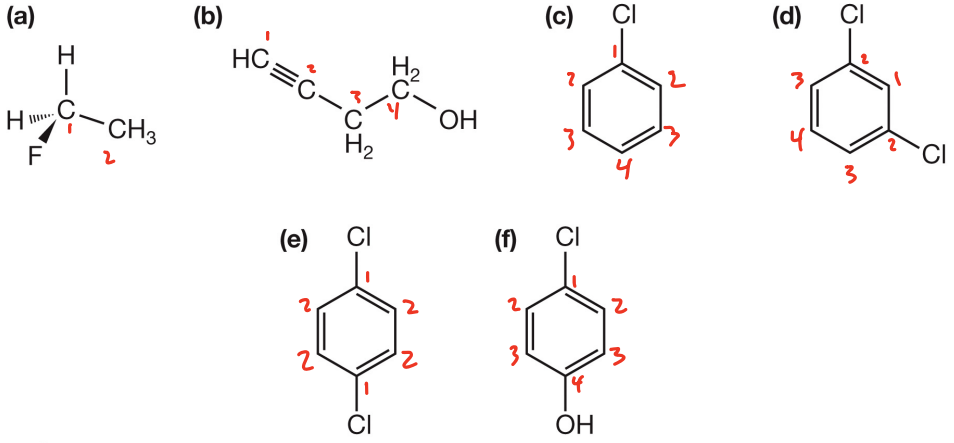
Chapter 17 Homework – Nuclear Magnetic Resonance (NMR)

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

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



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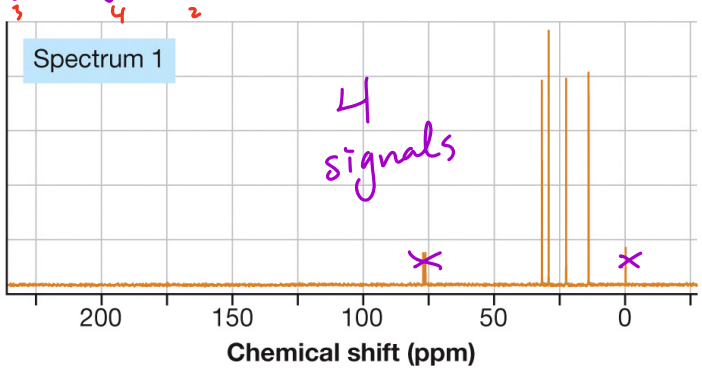
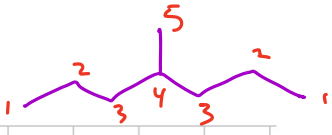
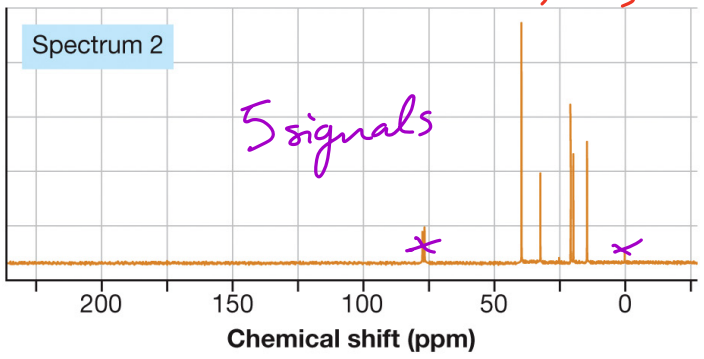
	Number of ^{13}C NMR signals
(a)	2
(b)	4
(c)	4
(d)	4
(e)	2
(f)	4

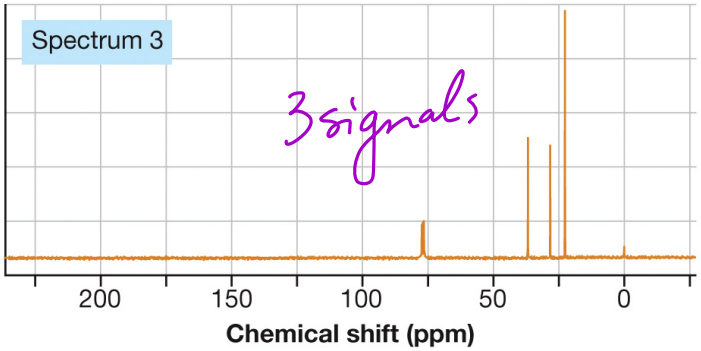
2. The ^{13}C NMR spectra of three isomers with molecular formula C_8H_{18} are given below. **Match each chemical name to its spectrum (1-3)**. Ignore the peak at 76 ppm (solvent).

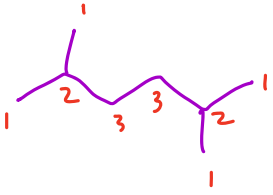
Isomer	Spectrum (1, 2, or 3?)
2,5-dimethylhexane	3
4-methylheptane	2
Octane	1











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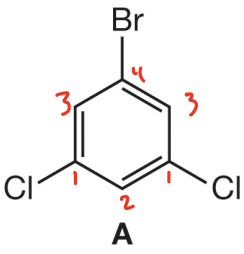
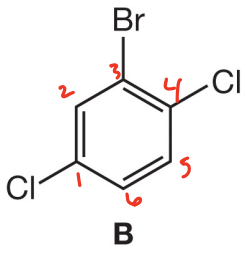
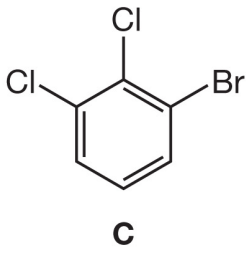
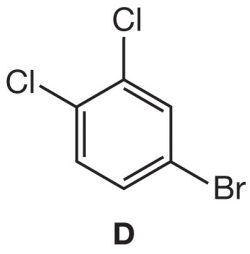
Ch 17A. ^{13}C NMR

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









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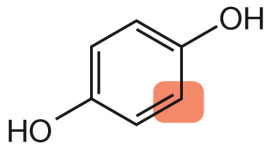
A	B	C	D
4	6	6	6

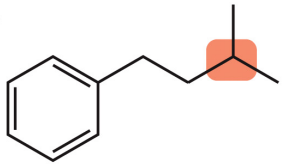
4. Indicate the **approximate chemical shift (range)** of each highlighted carbon in its ^{13}C NMR spectrum (Table 17-5).

(a)



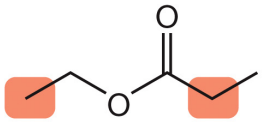
110-160 / CH

(b)



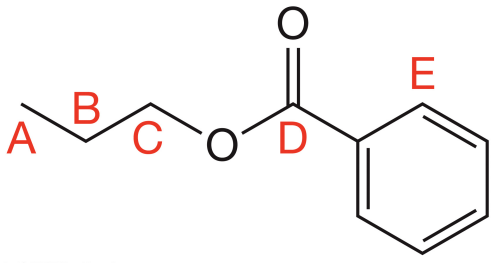
____ / CH

(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.



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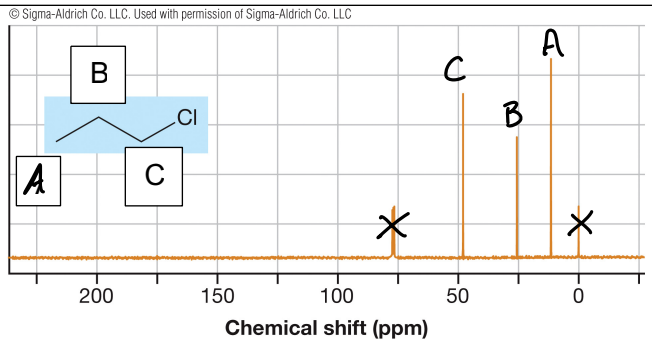
Signal	Chemical shift range (ppm) Karty Table 17-5	Mohrig NMR
A	10-25	7-30
B	20-45	15-40
C	55-70	55-80
D	160-185	160-180
E	128	110-160

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.

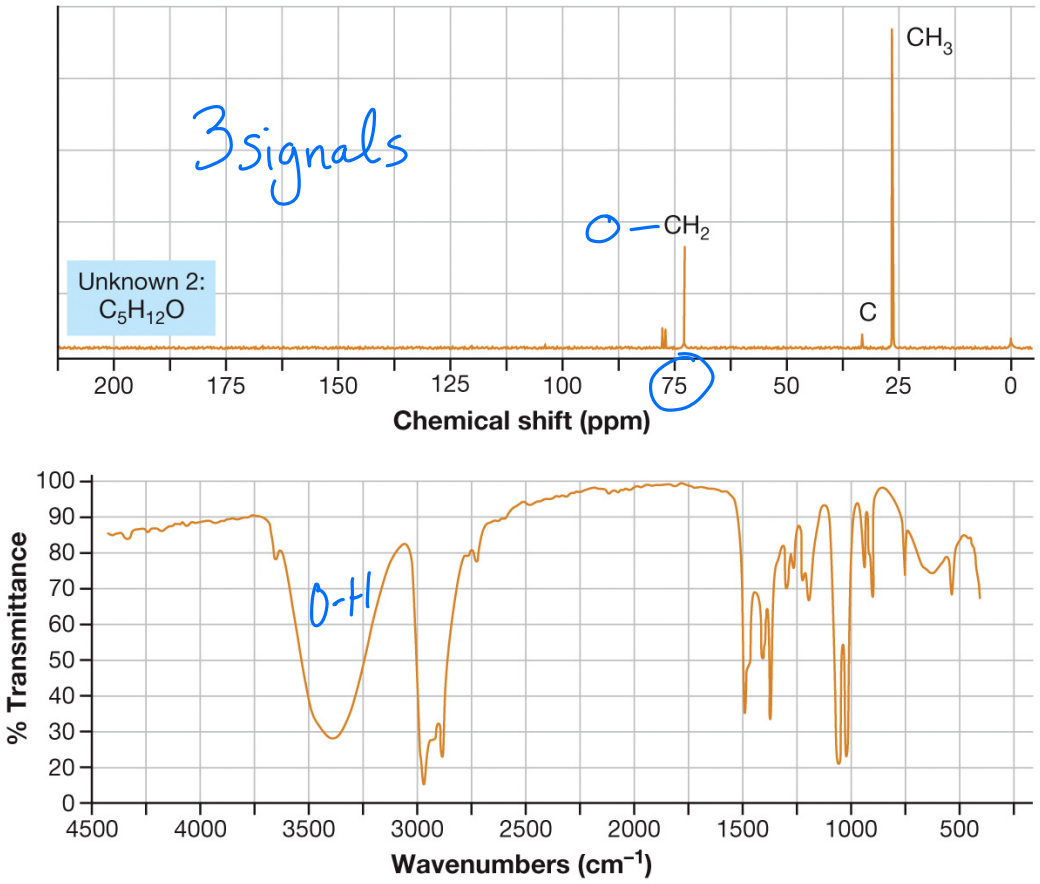


Signal (ppm)	Carbon (A, B, or C)
10	A
25	B
49	C

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

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

see class notes



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

O—CH2

5 C's, 3 signals → symmetry

C (no H's)

CH3

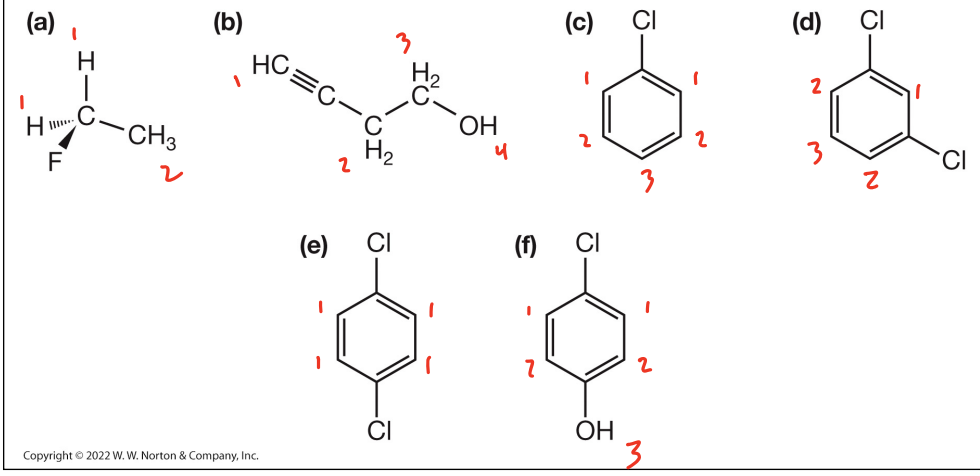
What clues does the **IR spectrum** provide about the structure?

alcohol O-H

Structure:

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

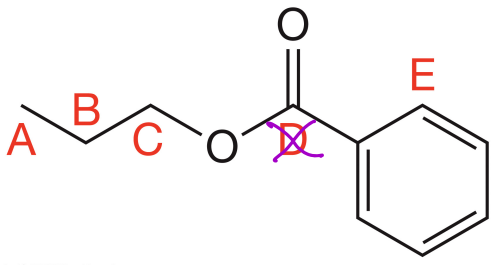
8. **How many signals** are expected in each compound's ^{1}H NMR spectrum?



	Number of ^{1}H NMR signals
(a)	2
(b)	4
(c)	3
(d)	3
(e)	1
(f)	3

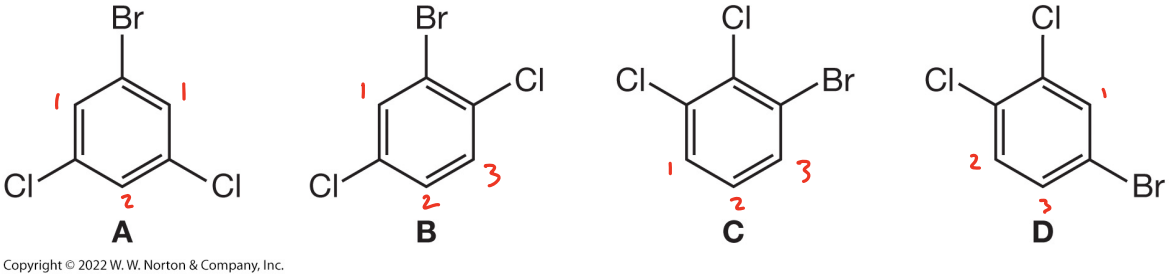
9. Indicate the **approximate ^{1}H NMR chemical shift** for each carbon (A-E) in the table below.

proton A-C, E



Signal	Chemical shift (ppm) Karty Table 17-1	Mohrig NMR
A	0.9	0.8-1.9
B	1.3	0.8-1.9
C	3.3	3.2-5.3
D		
E	7.3	6.9-9

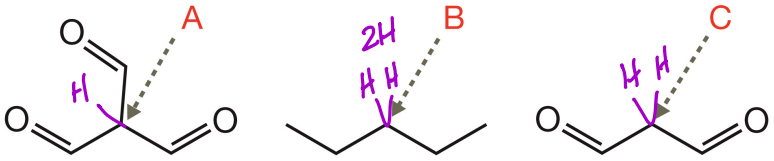
10. **How many signals** are expected in each compound's ^{1}H NMR spectrum?



A	B	C	D
2	3	3	3

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.



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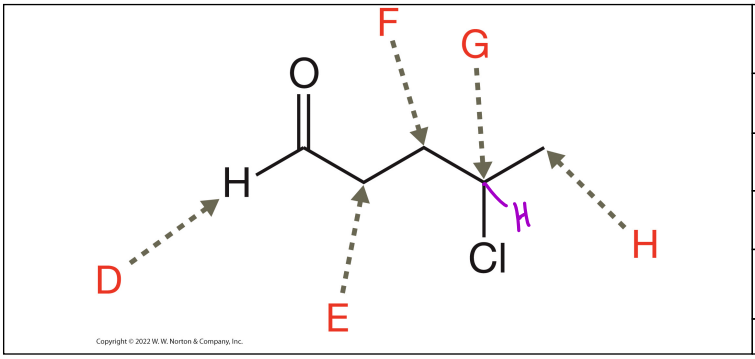
Chemical Shift Rank	Proton (A-C)	Integration (# of H's)
High	A	1H
Medium	C	2H
Low	B	2H

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.



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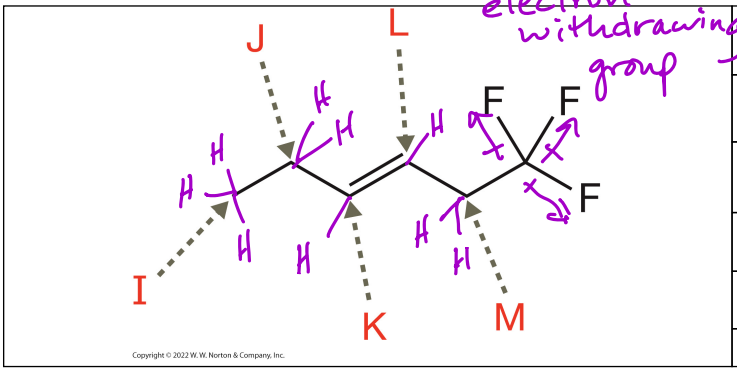
Chemical Shift Rank	Proton (D-H)	Integration (# of H's)
Highest	D	1
	G	1
close!	E	2
OK if switched	F	2
Lowest	H	3

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.

strong electron withdrawing group



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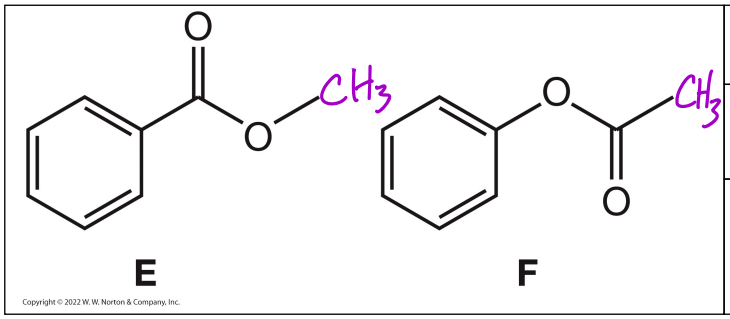
Chemical Shift Rank	Proton (I-M)	Integration (# of H's)
closer to CF_3 Highest	L	1H
	K	1H
	M	2H
	J	2H
Lowest	I	3H

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



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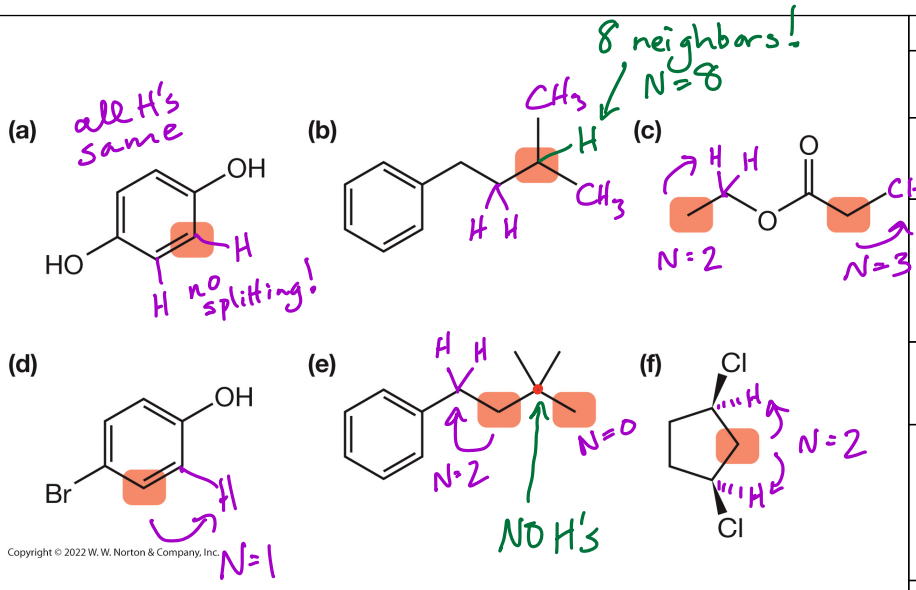
	Karty ^{1}H NMR (Table 17-1)	Mohrig	Karty ^{13}C NMR (Table 17-5)	Mohrig
E	3.3	3.2-5.3	55-70 C-O	55-80
F	2.1	1.9-3.3	not listed	30-45

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).



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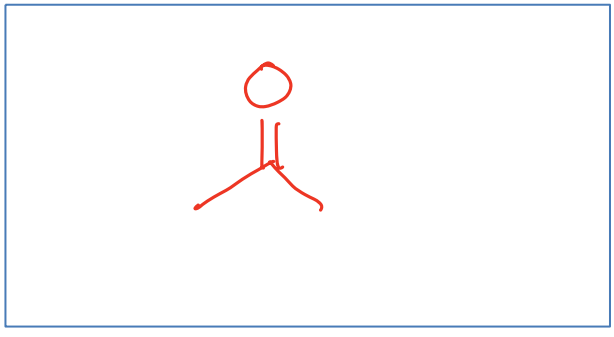
	Splitting Pattern(s) (N+1)
(a)	1, singlet
(b)	9, nonet
(c)	CH_3 group: 3, triplet CH_2 group: 4, quartet
(d)	2, doublet
(e)	CH_2 group: 3, triplet CH_3 group: 1, singlet
(f)	3, triplet

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

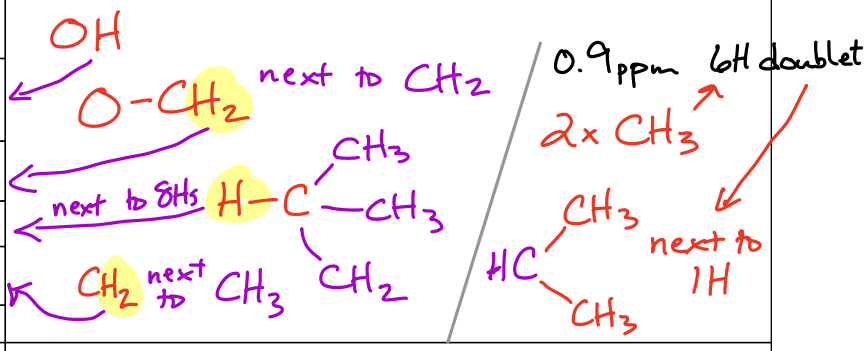
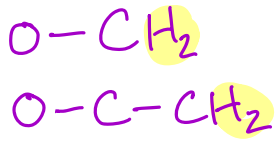
		What does each piece of data tell you about the compound?
Formula	C_3H_6O	Any double bonds? yes!
IR	1720 cm^{-1} (broad, strong) 2900 cm^{-1} (sharp, strong)	C=O C-H alkane
^{1}H NMR	One signal… Chemical shift = 2.0 ppm Integration = 6H Splitting = singlet	2x CH_3 O=C-CH_3
^{13}C NMR	? 207 ppm ? 31 ppm	C=O C-C=O

Structure:

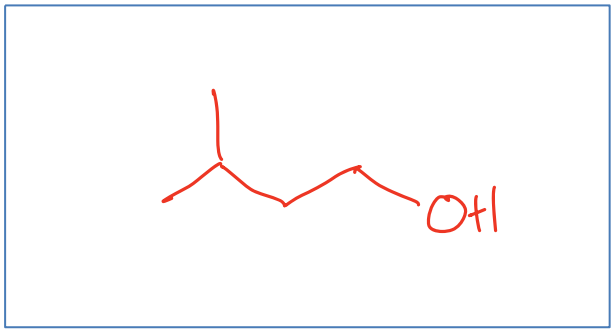


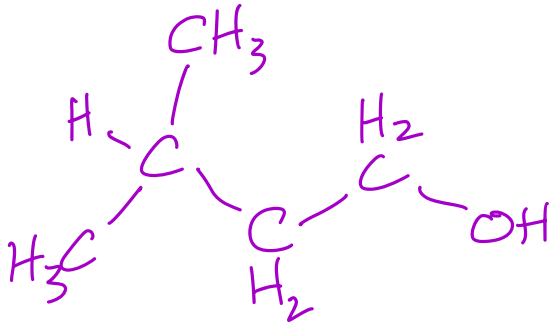
Chapter 17 HW

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

Formula	$C_5H_{12}O$ no double bonds 			**What does each signal tell you about the compound?** (show your work in the space below)
IR	3300 cm^{-1} 2900 cm^{-1}			OH C-H alkane
^{1}H NMR	**Chemical shift**	**Integration (# of Hs)**	**Splitting**	
	4.0 ppm	1 CH	Broad singlet	
	3.5 ppm	2 CH_2	Triplet	
	1.6 ppm	1 CH	nonet	
	1.5 ppm	2 CH_2	quartet	
	0.9 ppm	6 2xCH_3	doublet	
^{13}C NMR	? 61 (CH_2) close to O ? 42 (CH_2) kind close to O ? 25 (CH) ? 23 (CH_3) not close to O			

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!