Problem 13.1

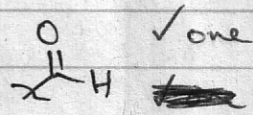
$C_7H_{12}O$

^{13}C NMR		^1H NMR
✓ 207, d	1	# 1.1, s, (6 H)
✗ 133, d	1	✗ 2.2, d, J = 7.2 Hz, (2H)
✗ 119, t	2	✗ 5.08, d, J = 11.8 Hz, (1 H)
✓✓ 46, s	0	✗ 5.11, d, J = 15.5 Hz, (1H)
42, t	2	5.75, ddt, J = 11.8 Hz, 15.5 Hz, 7.2 Hz (1H)
# 22, q (2)	6	✓ 9.5, s, (1 H)

IHD = 2 H's on C → all 12

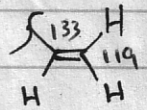
→ FG's

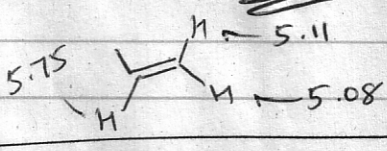
· 207 ^{13}C → Aldehyde ✓ → 9.5, s ^1H



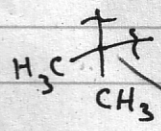
✓ one IHD

· 133, 119 → olefin ✗ vinyl (more later)





· 22 ^{13}C → two identical methyl groups # → 1.1 ^1H

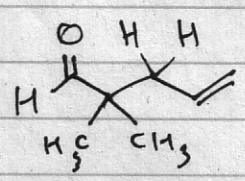


← Quaternary – know because of the singlet in ^1H NMR

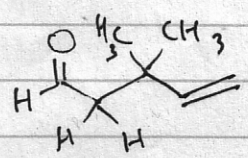
46 ✓✓

· only thing left is 42, t.

2 possible

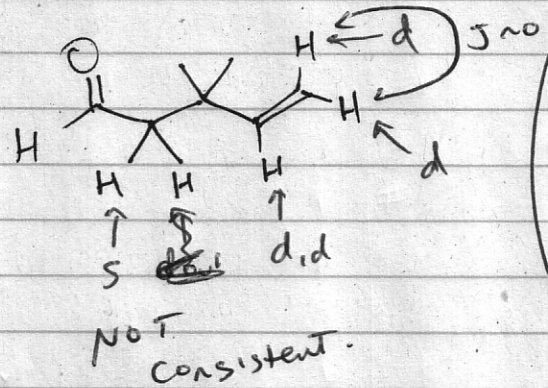


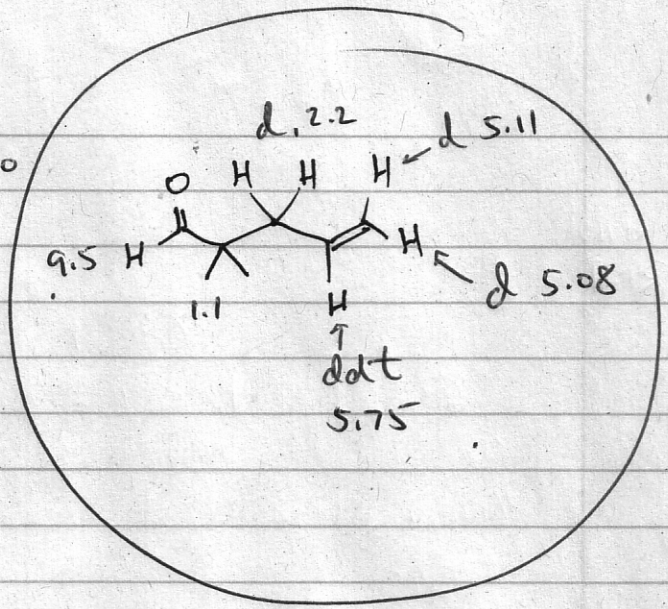
or



Problem 13.1 (cont')

expect

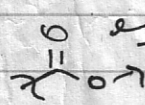




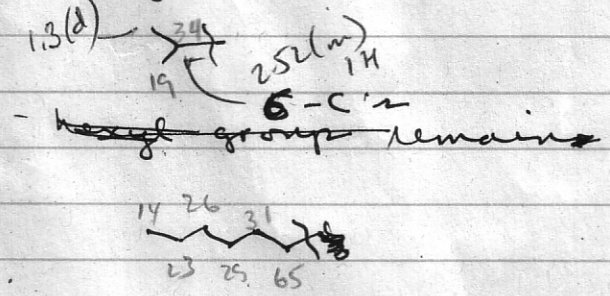
13.2 $C_{10}H_{20}O_2$

^{13}C		^1H NMR
✓ 177, s	HmC	0.9, t, J = 7.3 Hz, 3H
65, t	2	1.3, d, 6.5 Hz, 6H *
* 34, d	1	1.4 m, 6H
31, t	2	1.64 m, 2H
29, t	2	2.52, m, 1H *
26, t	2	4.05, t, J = 7.1 Hz, 2H.
23, t	2	
* 19, q (2)	6	
14, q	3	

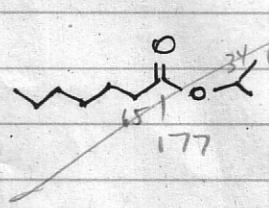
→ IHD = 1 ; H's on C : ALL

→  ester → ~~aldehyde~~

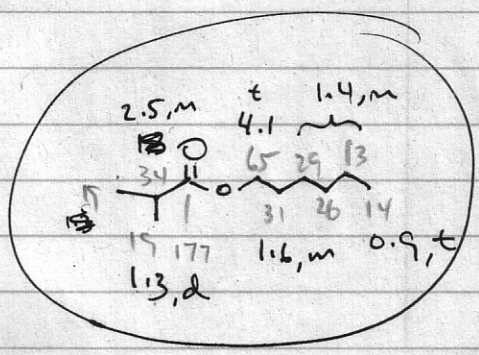
- methyl groups → yes - isopropyl *



- ~~hexyl group~~ remains

→ options 

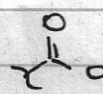
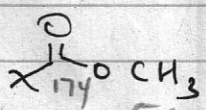
vs



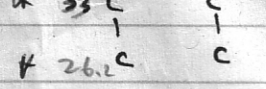
13.3 $C_6H_{16}O_2$

^{13}C NMR		^1H
✓174.n	0	3.67, s, 3H
✓51, q	3	2.12, d, J = 6.4 H_3, 3H
42, t	2	1.7, m, 6H
35, d	1	0.9 – 1.3, m, 5H
*33, t, 2C	4	
*26.2, t, 2C	4	
26.1 t	2	

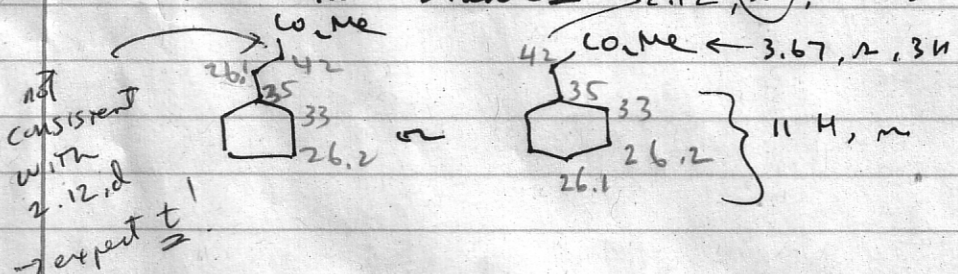
IHD = 2, H'n on C = All

FG'n  → Methyl ester  ✓

- No other FG'n → ring – NO other Me-groups
- * Symmetry in ring



- Fill in blanks → 2.12, (d), 2H.

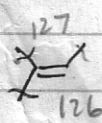


13.4 $C_8H_{11}N$

^{13}C			^1H
127.1	s		5.79, t, J = 6.2 Hz, 1 H
126.3	d	1	2.97, s, 2 H
117.7	s		2.02, m, 4 H
28	t	2	1.70, m, 4 H
26	t	2	
25	t	2	
23	t	2	
22	t	2	

→ IHD = 4, All H's on C

→ FG's? – Alkene – 2 C's.
– other is a nitrile



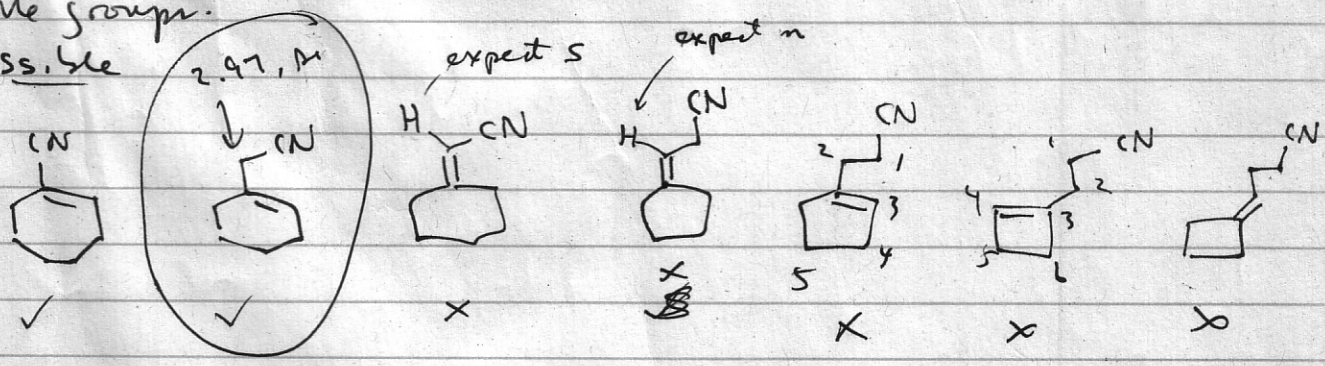
+C≡N
118

3 IHD's down.

Need ring | Frag. NC– 2.97, s, 2H

→ No Me groups.

→ Possible

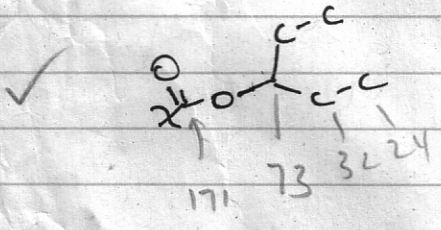


13.5 $C_8H_{14}O_2$

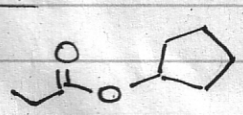
^{13}C		^1H NMR	
✓ 171, s	0	4.75, m, 1H	
✓ 73, d	1	2.03, s, 3H	
✓ 32, t (2 C's)	4	1.2-1.7, m, 10H	
25, t	2		
✓ 24, t (2 C's)	4		
22, q	3		
	14		

1 HD = 2, 4 on C all

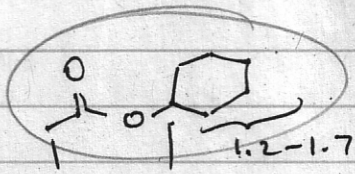
* ester → ring
→ look at connectivity & symmetry



Possible



would expect Ethyl-t, q



NOTE: ERRATA 2.52 - q not t.

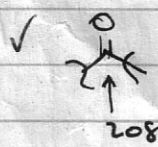
13.1

$C_8H_{17}NO$

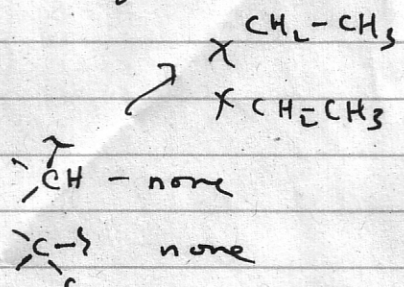
^{13}C		^1H
✓ 208, s	1	1.02, t, 7.1 Hz, 6H ✗
48, t	2	2.16, s, 3H
47, t	2	2.52, q, J = 7.1 Hz, 4H ✗
✗ ✓ 42, t, 2	4	2.61, t, J = 7.6 Hz, 2H
30, q	3	2.75, t, J = 7.6 Hz, 2H
✗ ✓ 12, q 2	6	
	17	

1 HD = ✗ 1

H's on C = all

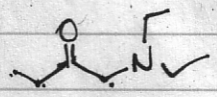
✓ 

✗ Symmetry

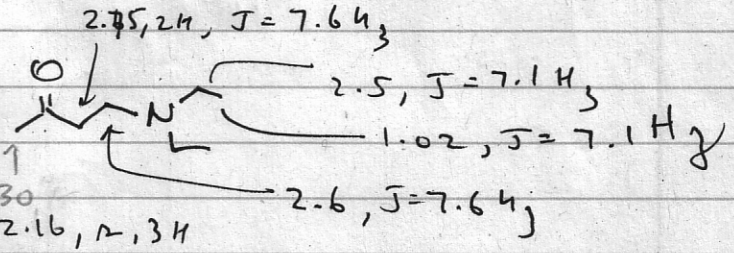


~~Left~~ Left w/ 2 triplets & a methyl.

options



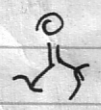
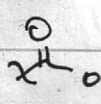
or



13.7 $C_8H_{12}O_3$

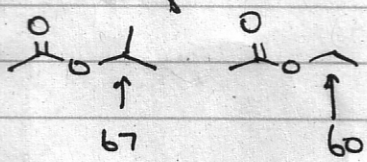
		^1H
✓ 212, s		* 1.28, t, J = 7.2, 3H
✓ 169, s		1.9–2.1, m, 2H
* 61, t	2	2.3, m, 4H
✡ 55, d	1	✡ 3.15, t, J = 8.4, 1H
38, t	2	* 4.2, q, J = 7.2, 2H
27, t	2	
21, t	2	
* 14, q	3	

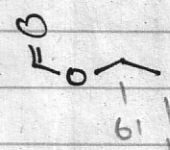
IHD = 3, H's on C - all

->   } 2 IHD's

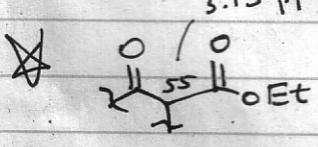
✓ ✓

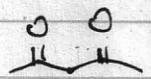
for comparison - ethyl ester not considered *





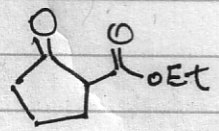
-> ring, no more methyls.



compare to 

(pg 123 of BCT)
(252 of OSSD)

~ full ring



13.8

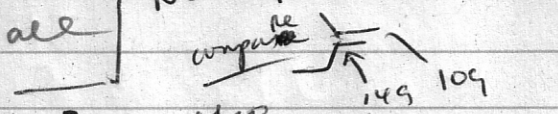
$C_6H_{11}NO_2$

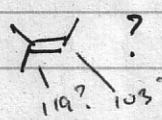
			^1H
✓	119, s	0	4.5, t, J = 6.2, 1H
*	103, d	1	3.4, s, 6H
✱	54, q (2)	6	2.4, t, J = 7.4, 2H
	29, t	2	1.92, dt, J = 6.2, 7.4, 2H
	12, t	2	

IHD = 2

H's on C – all

NO → BAD MATCH to TABLE 12.3 (BCT) pg 120 or C.3 (OSSD) pg 250



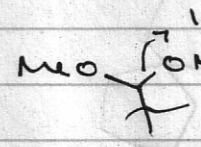
FG's → 

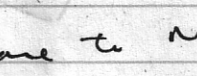
~~Also~~ can deal w/ the other IHD this way

What else:

✓ $C\equiv N$ – 119, s

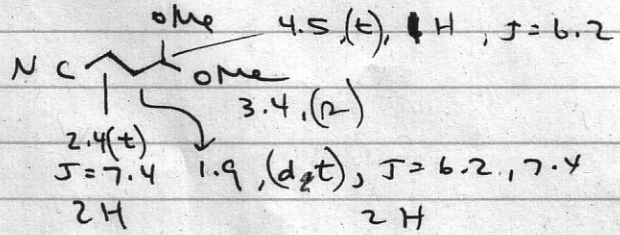
methyl group, symmetrical 54 → on oxygen

✱ H_3CO, OCH_3 => 

compare to 

pg 123 BCT
252 OSSD.

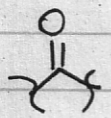
– No other Me-groups – FILL IN:



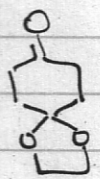
13.9 $C_8H_{12}O_3$

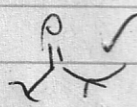
^{13}C	^1H
✓ 210 s	4.04, s, 4H
✗ 107 s	2.5, t, J = 6.6, 4H
✗ 64, t, 2 4	2.0, t, J = 6.6, 4H
38, t, 2 4	
34, t, 2 4	
all	

1 HD = 3

✓ 

✗ 

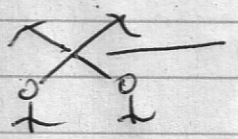
fill in 



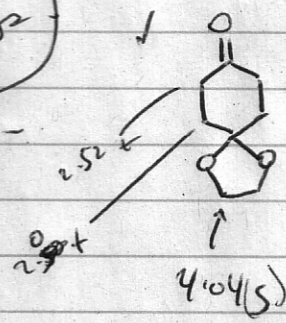
→ OTHER UNSAT? No → 2 rings

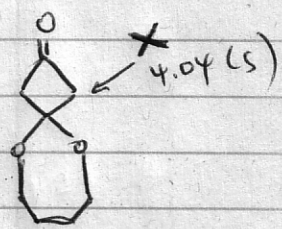
→ 3 symmetrical methylene –

→ other groups.

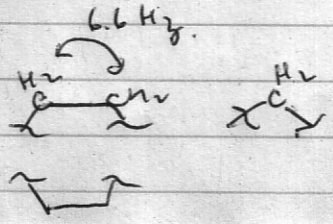


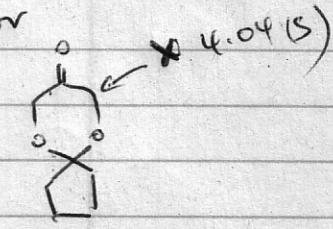
→ Fill in



or 

→ Look at J-coupling



or 

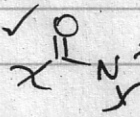
13.10

$C_9H_{17}NO$

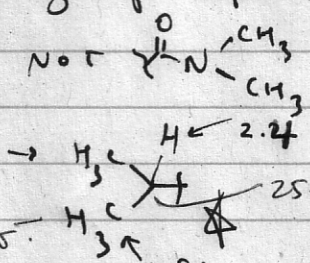
* Note: 3.44 = overlapping triplets
1.9 = overlapping app quintets

^{13}C NMR		^1H NMR	
✓ 171, s	0	0.96, d, J = 7.8, 6H	✡
* 47, t (2)	4	1.9, m, 4H	*
44, t	2	2.2, d, J = 6.8, 2H	○
* 26, t (2)	4	2.4, m, 1H	✡
✡ 25.5, d	1	3.44, m, 4H	*
✡ 23, q (2)	6		
	17 = all		

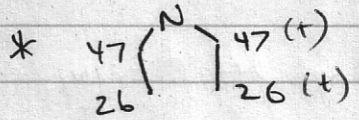
1 HD = 2

→ FG's: ✓  ; ring

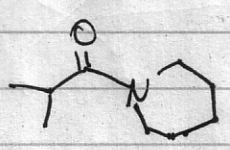
→ methyl groups → 23, q (6)



→ ATTACHED TO N



→ OPTIONS



or