P.S. #4 Answers

Chapt 4 #8: $C_5H_{12}O_2$ # sites of unsatn: $6-\frac{12}{2}=0$

only 3 ^{13}C resonances ∴ Some symmetry.

^1H NMR: integration 1:2:3 or 2:4:6

looks like CH_2 (not coupled) & CH_3-CH_2 (2x). } consistent with DEPT: two CH_2's & 1 CH_3

^{13}C signal shifts at 95 ppm

- looks like $O-CH_2-O$

Thus $CH_3-CH_2-O-CH_2-O-CH_2-CH_3$

Chapt 4 #9: $C_5H_{10}O$ # sites of unsat'n $6-\frac{10}{2}=1$

only 3 ^{13}C resonances ∴ Some symmetry.

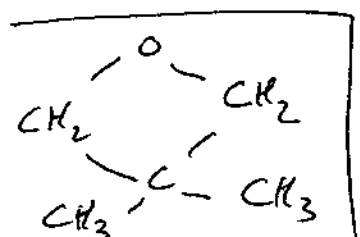
DEPT: CH_3 (26 ppm) $-\overset{|}{C}-$ (36 ppm).

CH_2 (8x)

^1H NMR $2CH_2-O$ + 2 CH_3 (not coupled)

no C=C's in ^{13}C - must be a ring.

So ⇒



P.S #4 Answers cont'd

Chap 4 #11: C_9H_8O # sites of unsat'n : $10 - \frac{8}{2}$

$= 10 - 4 = 6$

only 5 ^{13}C resonances ∴ symmetry.

Functional groups: ^{13}C at 215 ppm – $C(=O)$ (ketone).

^1H integration: ~7 ppm (4 H) – aromatic

3.5 ppm (4 H).

1 equivalent ∴ $2 \times CH_2$

^{13}C DEPT-135

CH_2 at 44

CH, CH at 125, 127, quaternary at 138.

1, 2

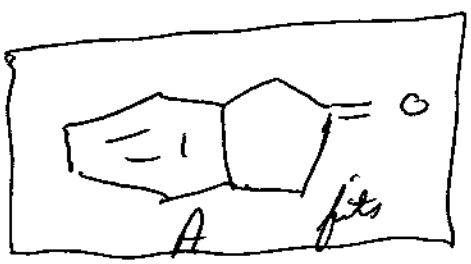
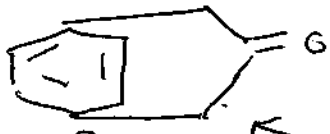
Rest 4 aromatic H's ∴  disubst'd

Can't be 1, 3 b/c ^1H spectrum

 a 

1, 3 1, 4

other site of unsat'n must be a ring.

So  or 

A fits B.

^{13}C expect 4 ∴ can't be this NOT

(C)

Chapt 4 #13: $C_7H_{12}O_2$ # sites of unsat'n:

$$8 - \frac{12}{2} = 2$$

7 ^{13}C resonances, ∴ NO SYMMETRY.

Functional groups: ^{13}C at 171 - looks like an ester

$$-\overset{O}{\overset{\|}{C}}-O$$

^{13}C's at 119 & 139 - indicate $C=C$

DEPT: CH_3 at 18, CH_3 at 21, CH_3 at 26

CH_2 at 61 CH at 119, $-\overset{|}{\underset{|}{C}}-$ at 139

From ^1H NMR coupling and integration information:

looks like $C=C(H)-CH_2$ ↑ doublet at 4.5

triplet at 5.5

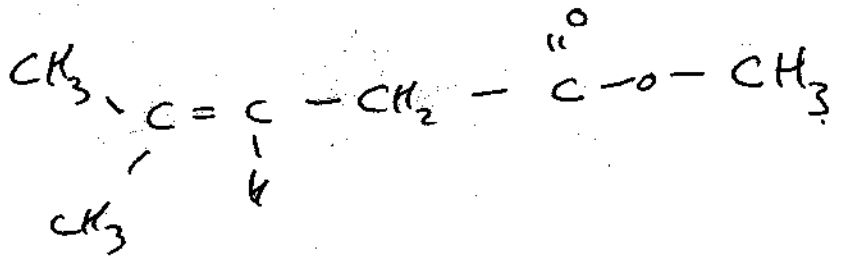
and 3 non coupled CH_3's, so all C's are accounted for.

Possible Structures:

I $\quad CH_3-C(CH_3)=C(H)-CH_2-O-\overset{O}{\overset{\|}{C}}-CH_3$

(D)

or

II. 

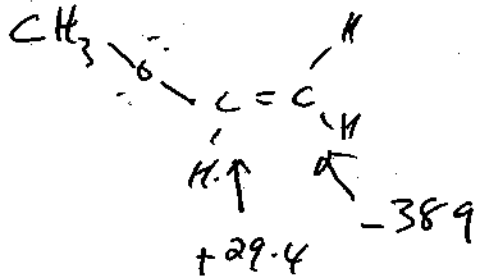
But structure II should have a 3 H singlet in ¹H nmr.

3.5 ppm — non exists.

also DEPT shows CH_2-O ↑ 61 ppm.

∴ I is a better fit & is correct.

Chpt 4 # 20: (a)



∴ predicted shifts are

+29.4

123.3

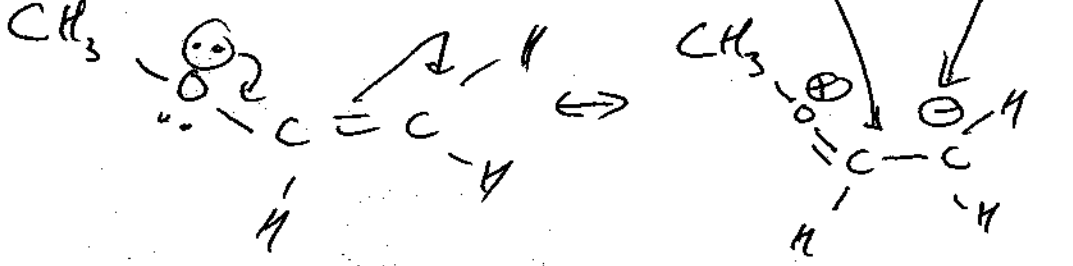
152.7

+ 84.4

Rationale:

deshielded

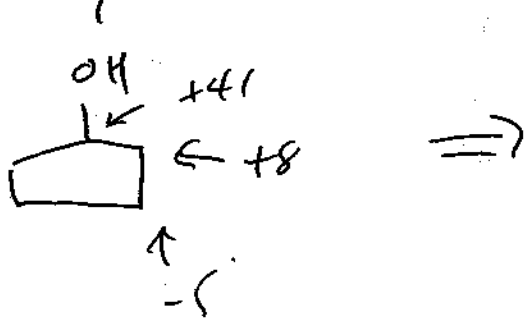
shielded!



(E)

Chapt # 20 (b)  is 25.6

using data in Table A8.3 : (internal OH effect)



20(f) $CH_3 - \underset{\underset{COOH}{|}}{CH} - CH_2 - CH_3$

butane central C is at 25.2 + terminal C is at 13.4

use COOH "internal" values

α	+16
β	+2
γ	-2

$CH_3 - \underset{\underset{COOH}{|}}{CH} - CH_2 - CH_3$

13.4 + 2 = 15.4

25.2 + 16 = 41.2

25.2 + 2 = 27.2

13.4 - 2 = 11.4