P.S. #5 ANSWERS

Chapt 5 #4: $CH_3-CH_2-C(=O)-CH=CH-CH_3$

(1) (2) (3) (4) (5) (6)

Analysis: 3H triplet at 0.88 ppm ("a") is CH_3 (1), split by CH_2 (2)

2H quartet at ~2.36 ppm ("c") is CH_2, split by CH_3.

^3J occurs 5 times in the spectrum – take the average value.

ie

271.14	263.88	719.42	712.02	704.76
263.88	256.47	712.02	704.76	697.35
7.26	7.41	7.40	7.26	7.39

average = 7.34 Hz

For the "b" protons (3H d, d at 1.7 ppm): must be CH_3 - split by ^3J to H_5 + ^4J to H_4 ie "tree"

^4J is

513.06	506.24
511.43	504.61
1.63	1.63

1.63 Hz

^3J is

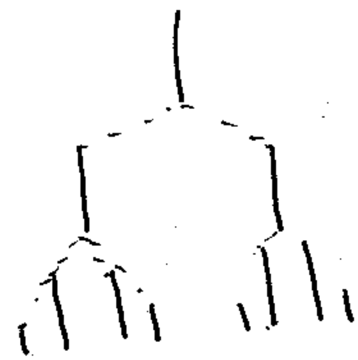
513.06	511.43
506.24	504.61
6.82	6.82 Hz

Chapt 5 #4 cont'd

Both H_4 + H_5 are doublets of quartets,
∴ they couple to each other + to the CH_3.

But, since $^3J > {}^4J$, H_5 must be at ~ 6.68 ppm
& H_4 " " " ~5.92 ppm

"tree" for H_5 + for H_4



^3J occurs 6 times here

^4J occurs 6 times here

ie. 216.57 − 209.75 = 6.82 etc

1787.54 − 1785.91 = 1.63 etc.

Also ^3J between H_4 & H_5 occurs 8X in the spectrum

ie 2016.57 − 2002.94 = 13.63

2009.75 − 1996.12 = 13.63 etc!

∴ $^3J_{4,5} = 13.63$ — consistent with (H)C=C(H)

Chapt 5 #16: From ^{13}C DEPT-135:

- CH_3
- CH_2
- CH_2
- CH – aromatic
- quaternary
- CH – aromatic
- quat
- quat

only 8 peaks ∴ symmetry.

$C_{10}H_{12}O_3$:

$DBE = 11 - \frac{12}{2} = 6$

from ^1H:

CH_3-CH_2-O — CH_3 at 1.4 (triplet), CH_2 at 4 ppm (quartet).

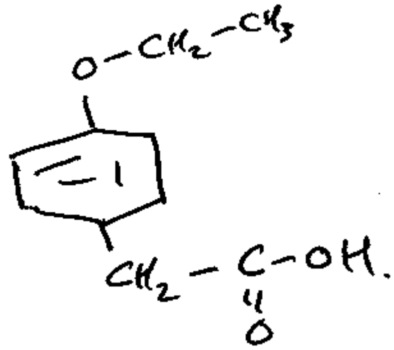
$-CH_2-$ — no adjacent protons @ 3.5

+ $C(=O)-OH$ — 12.5 ppm

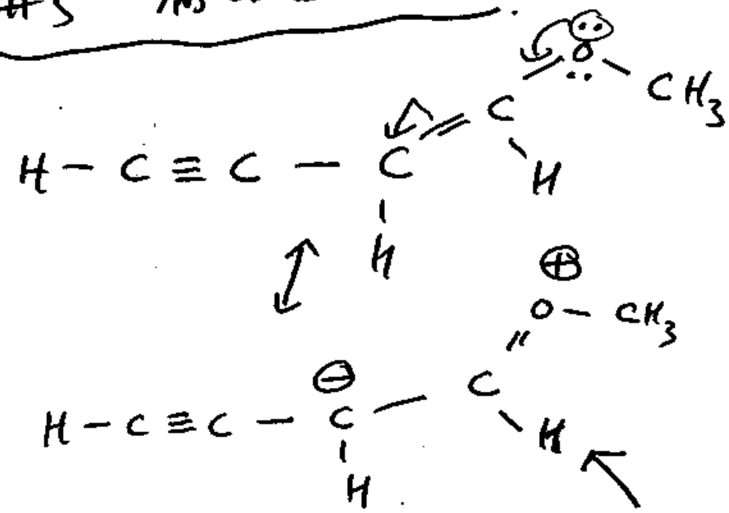
and a para-disubstituted aromatic ring from doublets and 7 ppm

^{13}C chemical shifts: only one CH_2-O — 63 ppm

Best structure is



Chapt 5 #20:



Assignment: H(d) is most deshielded ∴ of above

So for this proton (at ~ 6.40 ppm)

Couplings are:

$1923.24 - 1922.76 = .48$

$1917.24 - 1916.76 = .48$

$1923.24 - 1917.24 = 6.0$

$1922.76 - 1916.76 = 6.0$

0.48 + 6.0 Hz

for proton at 4.60 ppm (H_c)

J's are

$1384.50 - 1381.50 = 3.00$

$1378.50 - 1375.50 = 3.0$

and

$1384.5 - 1378.5 = 6.0$

ie 3.0 and 6.0 Hz

Chapt 5 #20 cont'd:

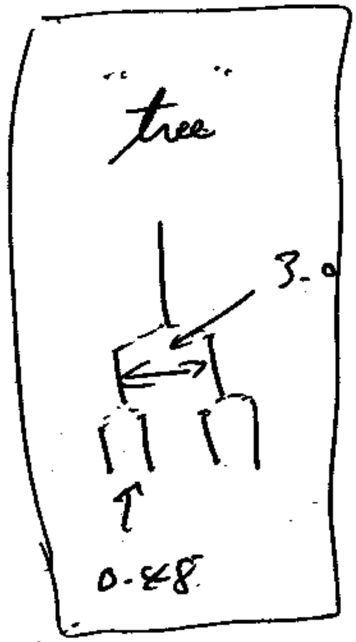
for H_a (at ~3.10 ppm)

J's are

$$931.77 - 931.25 = 0.48 \qquad 928.77 - 928.25 = 0.48$$

and

$$931.77 - 928.77 = 3.0 \qquad 931.25 - 928.25 = 3.0$$

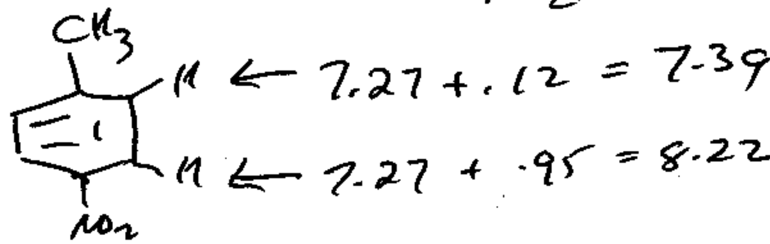


ie 0.48 + 3.0 Hz

Chapt 5 #32 (a)

alkyl	NO_2	
-0.14	0.26	⇒ +.12
-0.06	0.95	⇒ +.89

so



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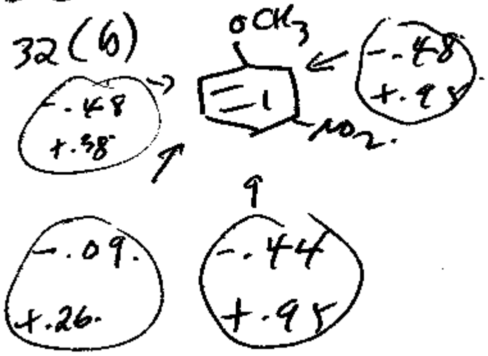
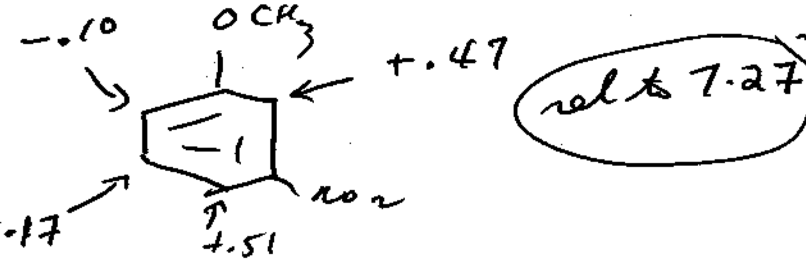
32 (b)



OCH_3

NO_2
ortho +.95

so



(rel to 7.27)