Problem Set #3 Answers:

Chapt 3 #2: (a) Since $\nu = \frac{\gamma B_0}{2\pi}$, there is a linear relationship between field strength B_0 and resonance frequency ν.

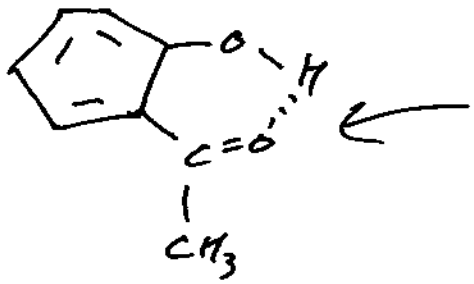
$\therefore$ the proton will be $\frac{2.82}{1.41} \times 90 = 180$ Hz downfield from TMS.

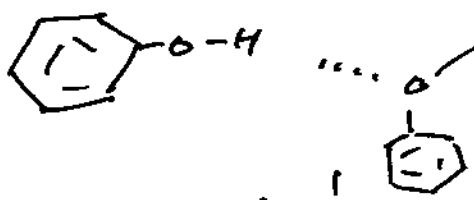
(b) Chemical shift is always the same in ppm.

$\therefore$ at 60 MHz $\delta = \frac{90}{60 \times 10^6} = 1.5$ ppm

and at 120 MHz $\delta = \frac{180}{120 \times 10^6} = 1.5$ ppm.

Chapt 3 #5: In ortho-hydroxy acetophenone, the O–H is intra molecularly hydrogen bonded

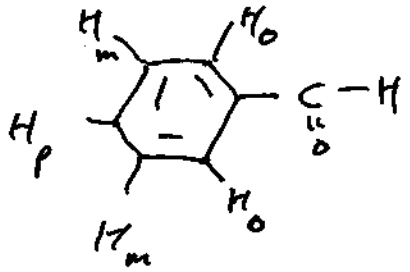
ie  ← Thus little conc'n dependence

But in phenol,  intermolecular,

$\therefore$ depends on concentration!

Problem Set #3 Answers

Chapt 3 #7:



The chemically equivalent ortho H's are deshielded by the C=O, ∴ at 7.87 ppm.

Hm's & Hp are chemically different, but only small chemical shift difference, since remote from c=o group.

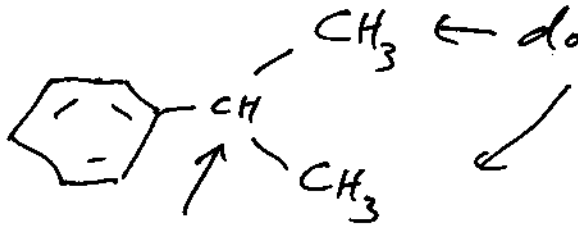
Chapt 3 #13

$CH_3 - CH_2 - CH_2 - Br$

- CH_3: triplet at ~1 ppm
- CH_2 (middle): triplets & quartets at ~1.5 ppm
- CH_2 (Br): triplet at ~3 ppm (range 2.7 → 4.1 ppm).

Chapt 3 #15: C_9H_{12} # sites of unsat'n = $\frac{10-12}{2}$ = 4

looks like



Problem Set #3 Answers

Chapt 3 #16: $C_4H_7O_2Br$ # sites of unsaturation: $5 - \frac{7}{2} - \frac{1}{2} = 1$

Since $-\overset{\overset{O}{\|}}{C}-O-H$ is present,

looks like $CH_3-CH_2-\underset{\underset{H}{|}}{\overset{\overset{Br}{|}}{C}}-\overset{\overset{O}{\|}}{C}-OH$

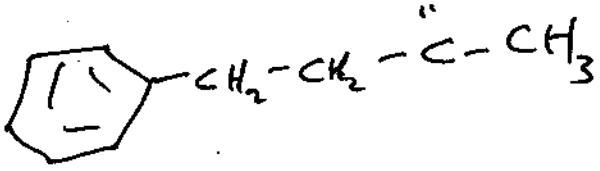
- CH_3: triplet at 1 ppm
- CH_2: doublet of quartets
- CH: ← triplet at 4.1
- complex at 2.0

Chapt 3 #24(b): Integration shows 5 aromatic H's (7.1 → 7.3 ppm)

2 H triplet – 2.8 ppm
2 H triplet – 2.9 ppm
} ∴ $-CH_2-CH_2-$

$C_{10}H_{12}O$ # units of unsat'n = $11 - \frac{12}{2} = 5$

the CH_3 singlet near 2 ppm (maybe $\overset{\overset{O}{\|}}{C}-CH_3$)

Looks like: 

Problem Set #3 Answers

Chpt 3 #27: $C_5H_6O_2$: # units of unsat'n

$= 6 - \frac{6}{2} = 3$

looks like: $O-CH_2-CH_3$ must be present
$C=O$ ↑ quartet at ~4 ppm

keys with: C_2H ∴ must be

$H-C\equiv C-\overset{O}{\overset{\|}{C}}-O-CH_2-CH_3$

↑ singlet at ~3 ppm.

Chpt 3 #28: $C_7H_{12}O_4$ # units of unsat'n $= 8 - \frac{12}{2} = 2$

Integration: ratio 2 : 1 : 3 ← 1.2 ppm
↑ 4 ppm ↑ 3 ppm

∴ must be symmetrical! 4H, 2H, 6H

must also have $O-CH_2-CH_3$
↑ 4 ppm quartet

IR: ester ∴ diester

$CH_3-CH_2-O-\overset{O}{\overset{\|}{C}}-CH_2-\overset{O}{\overset{\|}{C}}-O-CH_2-CH_3$!