#64 on Structure Elucidation Website

$C_{10}H_{12}O$

$C_nH_{2n+2+N-X}$

$H_{2(10)+2+0-X} = H_{22}$

$-H_{12}$

2 | 10 Missing hydrogens

→ 5 units of unsat

High # of units & Low # of Carbons = Aromatic Ring

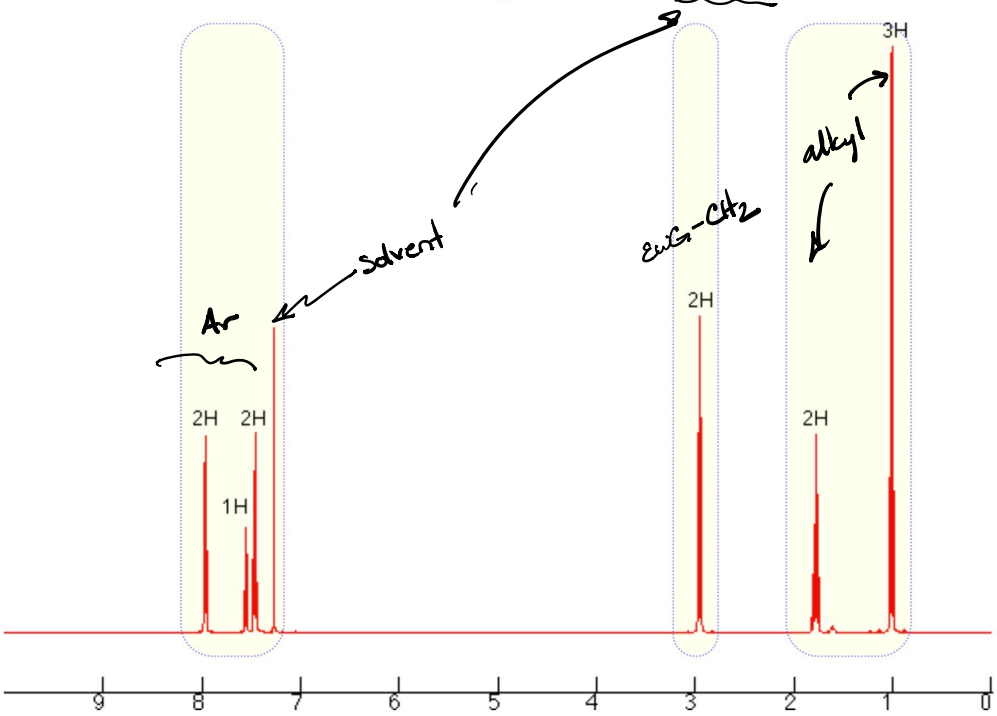
≥4 ≤12

 = 4 units

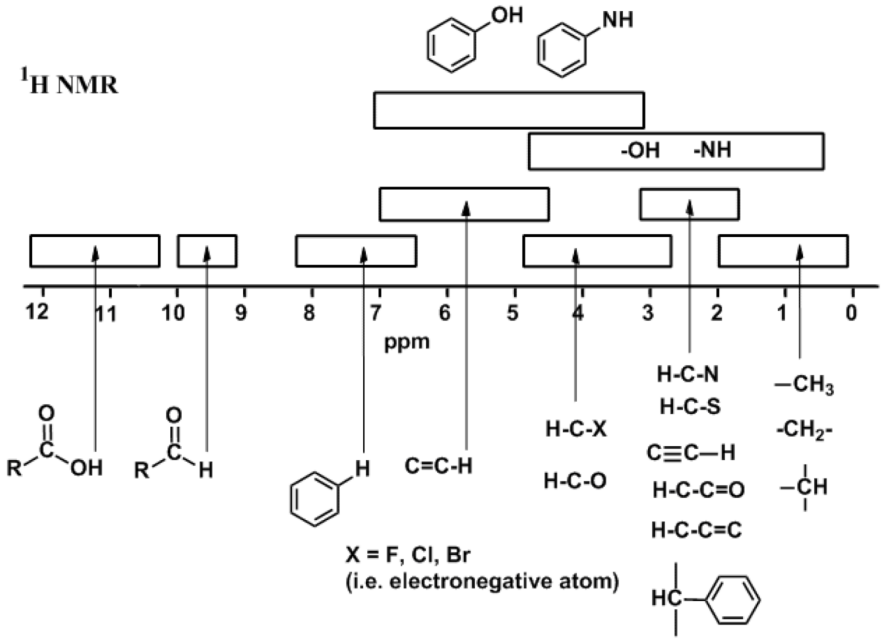
$C_{10}H_{12}O$ =  + 1 ring or alkene or 

4 units ?

Problem 64 - ^{1}H NMR spectrum ($CDCl_3$, 500 MHz)

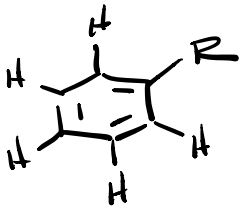


Click on the highlighted area to zoom. Click again to zoom back out.

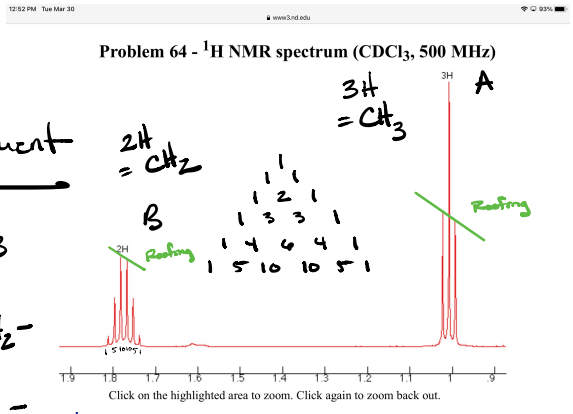


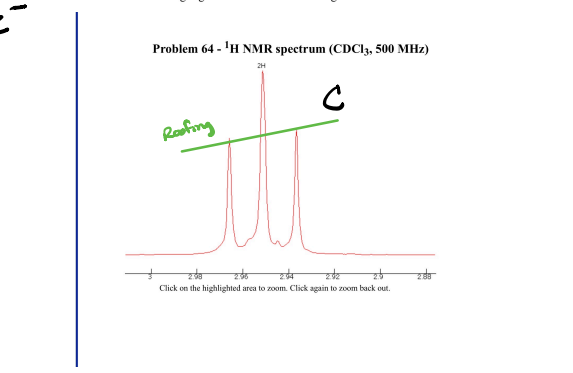
HNMR Data Table

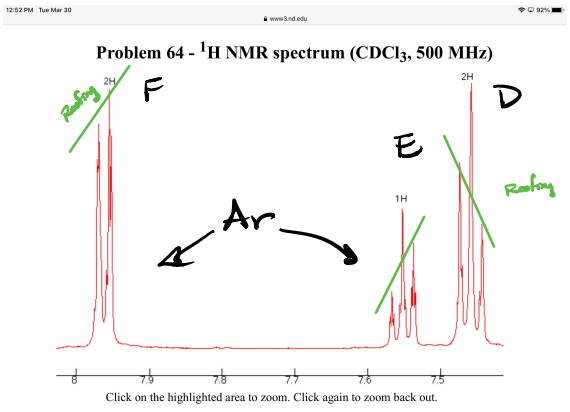
	ppm	Int	Mult	# of Neighbors	Assignment
A	1.0	3	t	2	$-CH_3$
B	1.8	2	sextet	5	EWG $-CH_2-$
C	3.0	2	t	2	strong EWG $-CH_2-$
D	7.5	2	t	2	Ar
E	7.55	1	t	2	Ar
F	8.0	2	d	1	Ar



Monosubstituted







strong EWG $-CH_2-$

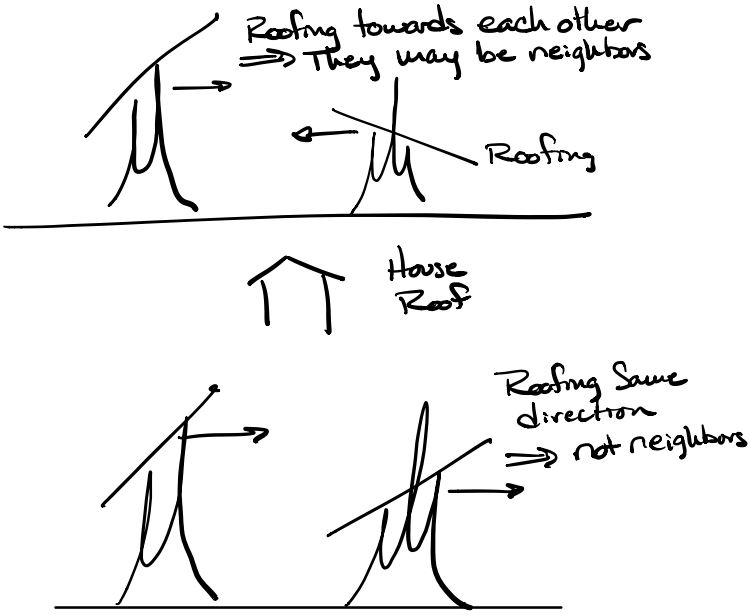
EWG $-CH_2-$

$-CH_3$

C_9H_{12}

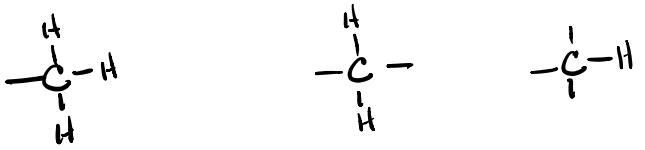
$C_{10}H_{12}O$

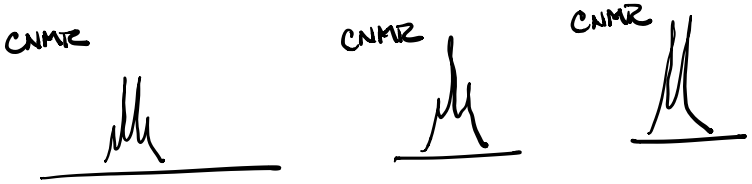
missing CO

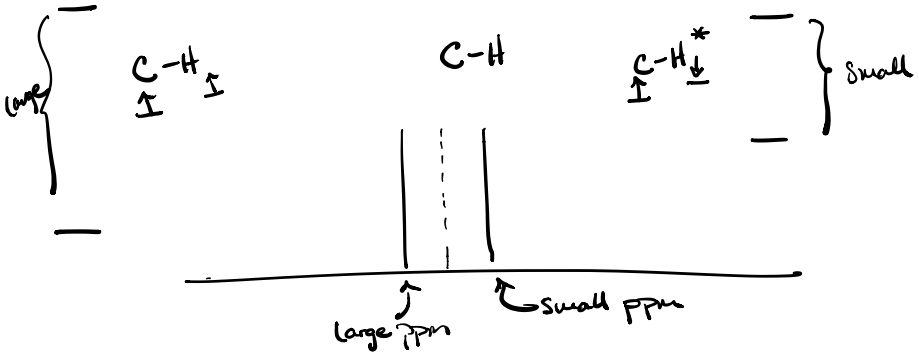

Roofing towards each other
⇒ They may be neighbors
Roofing
House
Roof
Roofing Same
direction
⇒ not neighbors

^{13}C NMR

C–H The hydrogen splits the carbon







Decoupling Experiment

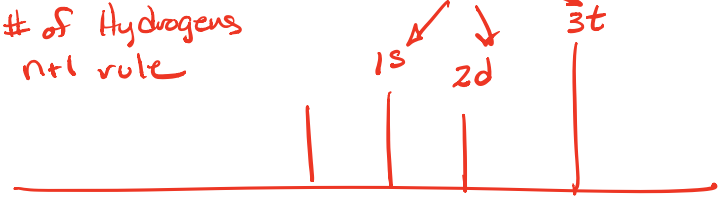
^{1}H-NMR fast pulse → H* ↓ 100% excited state

H* ↓
H ↑ } ~50/50 @ Room Temp

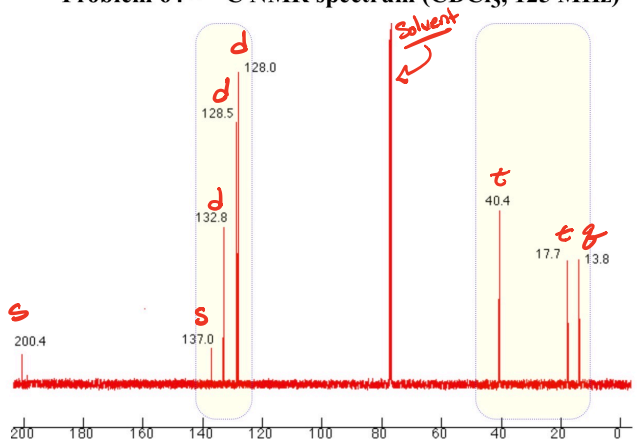
Almost All ^{13}C NMR is decoupled. Special Experiments are done to get the coupling data

Coupling data w/ proton

Gives # of Hydrogens through n+1 rule



Problem 64 - ^{13}C NMR spectrum ($CDCl_3$, 125 MHz)



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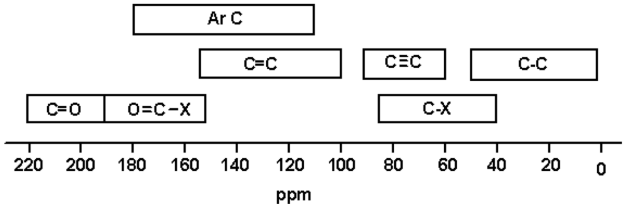
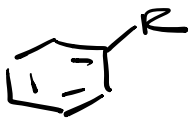


CNMR Data table

ppm	mult	# H's	Assignment
13.8	q	3	$-CH_3$
17.7	t	2	EWG $-CH_2-$
40.4	t	2	Strong EWG $-CH_2-$
128	d	1	Ar-H 
128.5	d	1	
132.8	d	1	
137.0	s	0	Ar 
200.4	s	0	 EWG

From ^{1}HNMR



$-CH_3$

EWG $-CH_2-$

Strong EWG $-CH_2-$

From ^{13}CNMR

$-CH_3$

EWG $-CH_2-$

Strong EWG $-CH_2-$

 = EWG

$C_{10}H_{12}O$ ✓

From ^{1}HNMR Multiplicity

$-CH_3$ Has 2 neighbors

EWG $-CH_2-$ Has 5 neighbors

Strong EWG $-CH_2-$ Has 2 neighbors

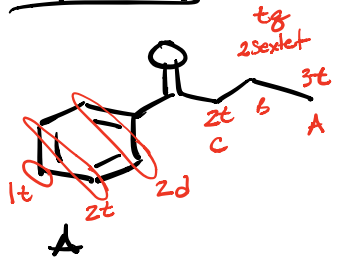
EWG $-CH_2-CH_2-CH_3$

CH_2: t

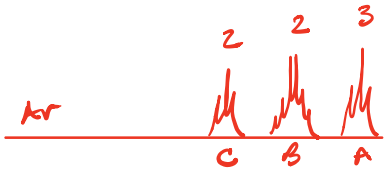
CH_2: sextet

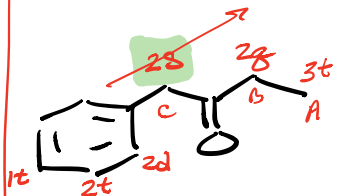
CH_3: t

Options

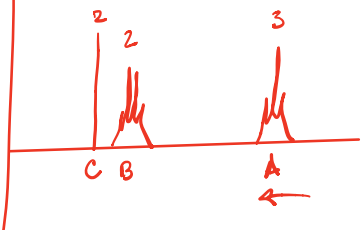


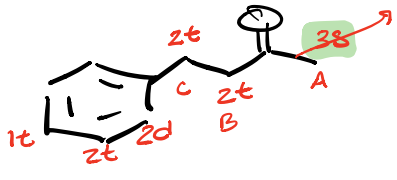
A



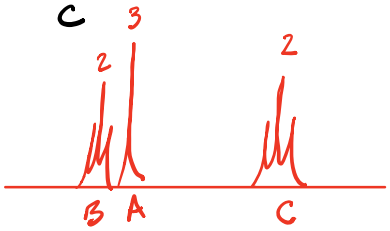


B

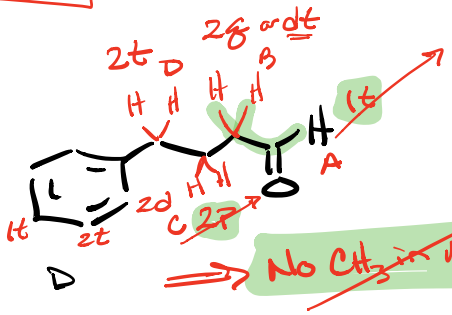




C

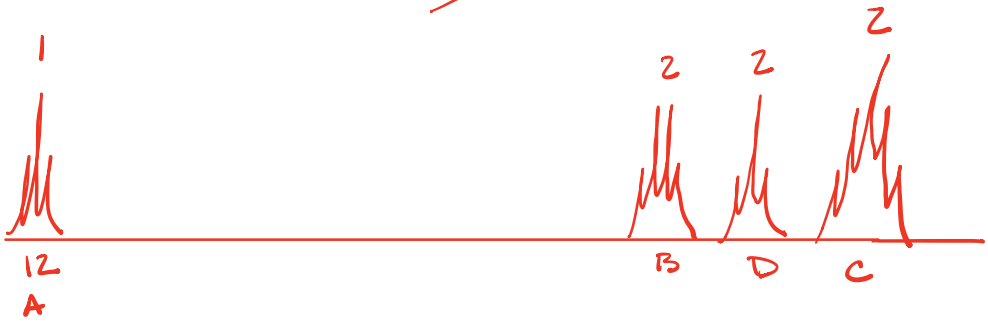


Fits Data

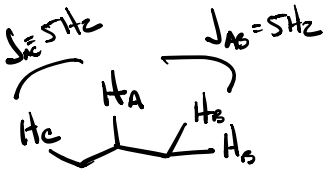


D

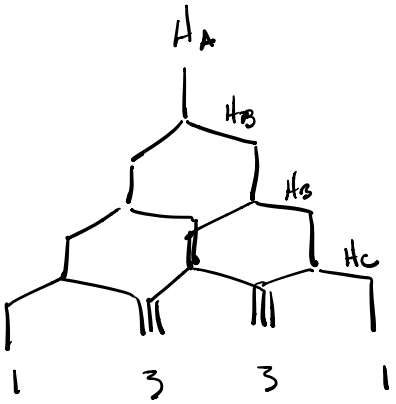
No CH_3 in Molecule

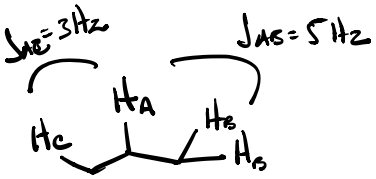


quartet or double triplet



3 neighbors all same J value





2 + 1
↓ ↓
t d = dt