#64 on Organic Structure Elucidation

$C_{10}H_{12}O$

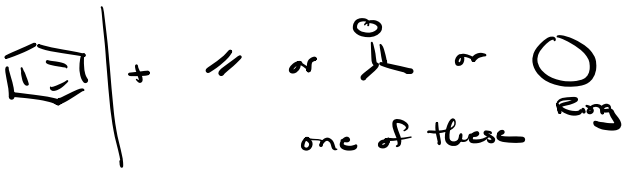
$2(10)+2 = 22$

-12

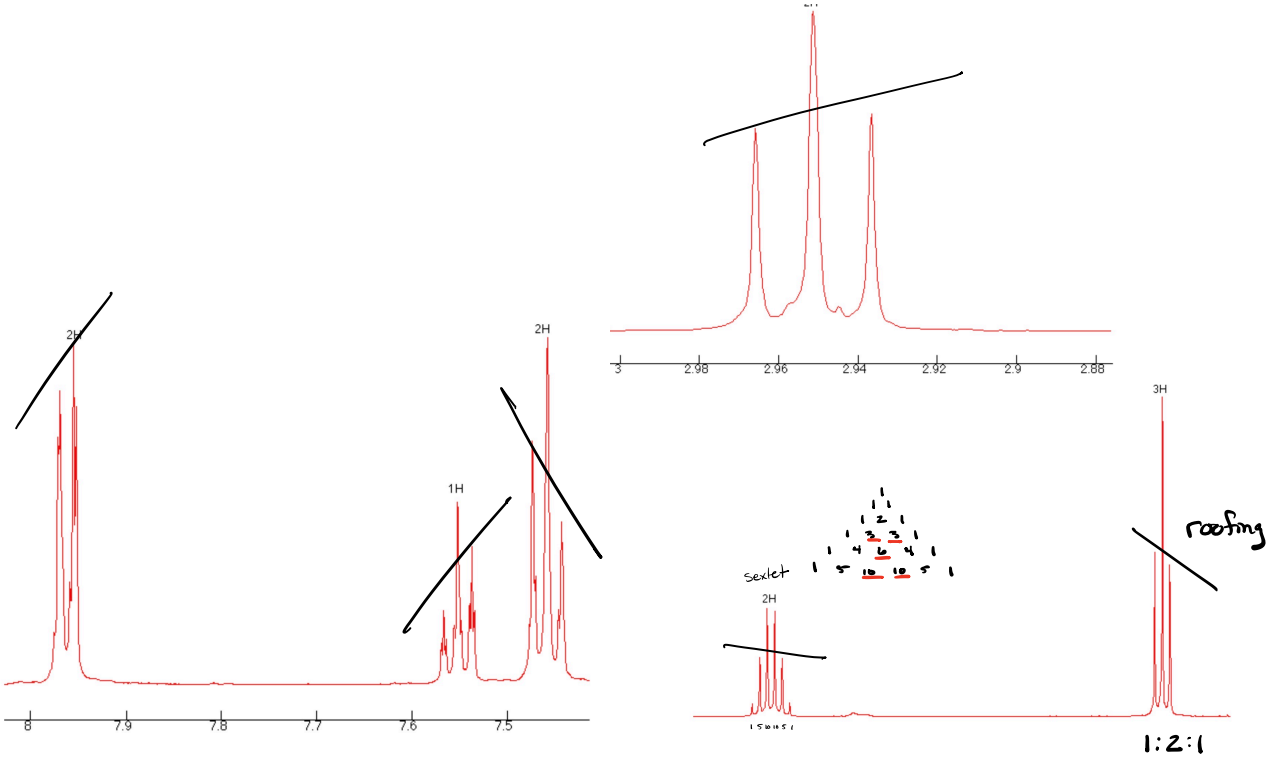
$2\overline{)10}$

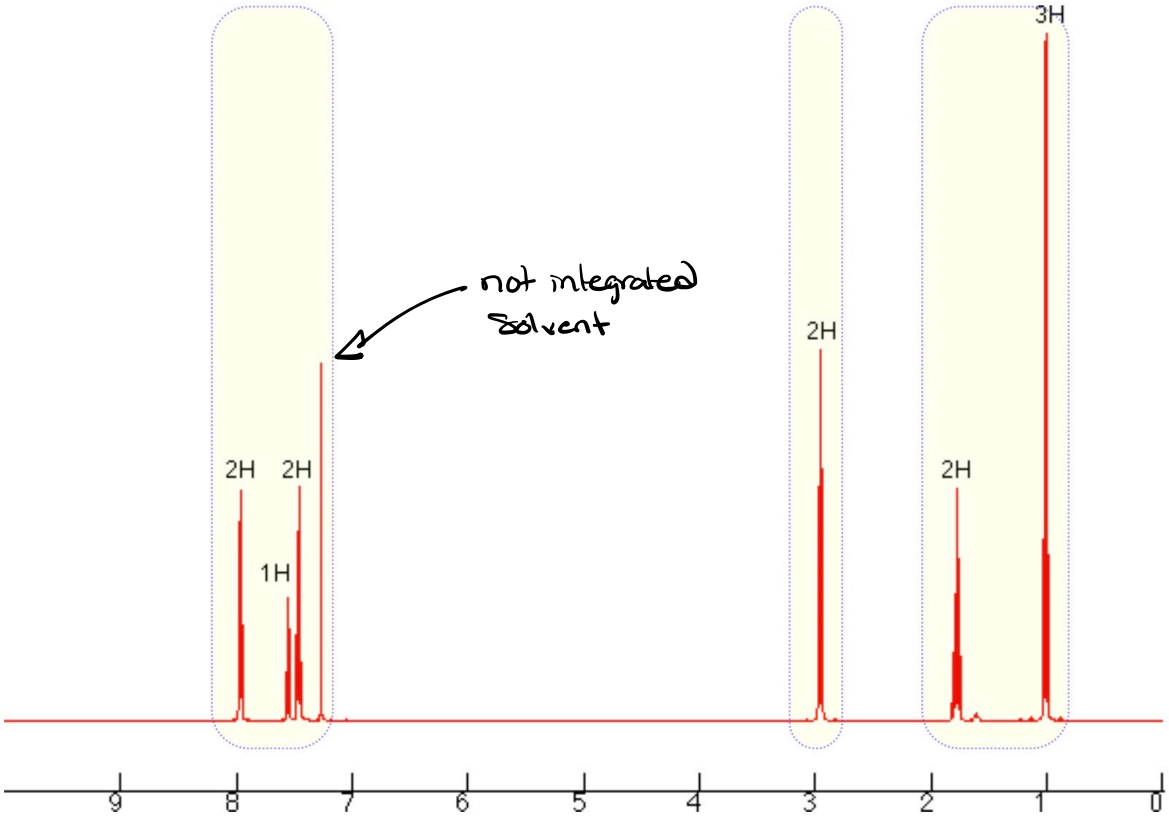
5 units unsat

Anytime ≥ 4 units $\Rightarrow$ Aromatic



one of these



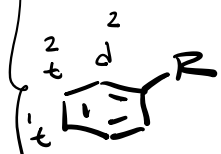


Click on the highlighted area to zoom. Click again to zoom back out.

^{1}H-NMR # environments = 6

n+1 Rule (−1)

ppm	Int	mult	#neighbors	Assignment
1.0	3	t	2	CH_3-
1.9	2	sextet	5	$CH_2-CH_2-CH_3$
3.0	2	t	2	$EWG-CH_2-CH_2$
7.4	2	t	2	Ar
7.5	1	t	2	Ar
8.0	2	d	1	Ar
	5			



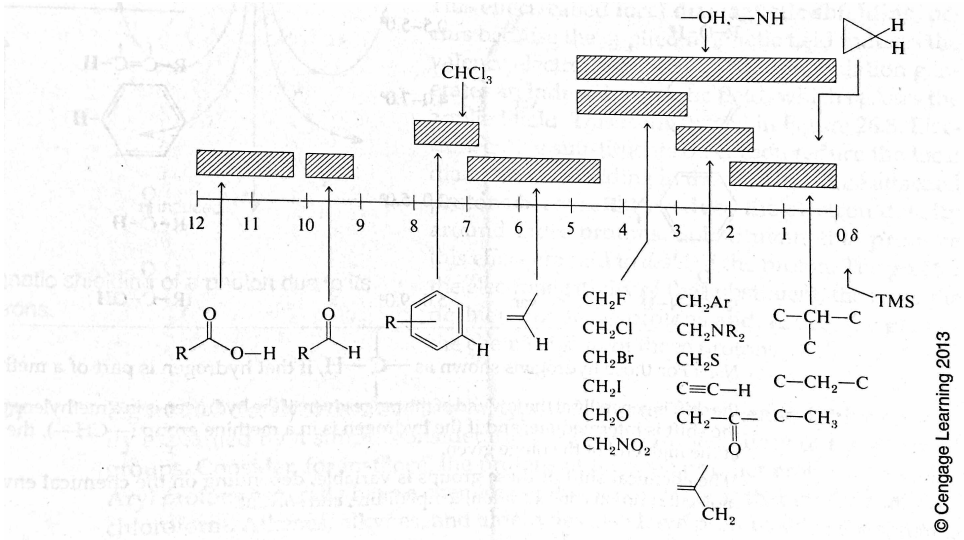


Figure 26.7
A simplified correlation chart for proton chemical shift values.

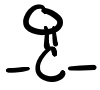
Ex: $CH_2-CH_2-CH_3$

C_9H_{12}

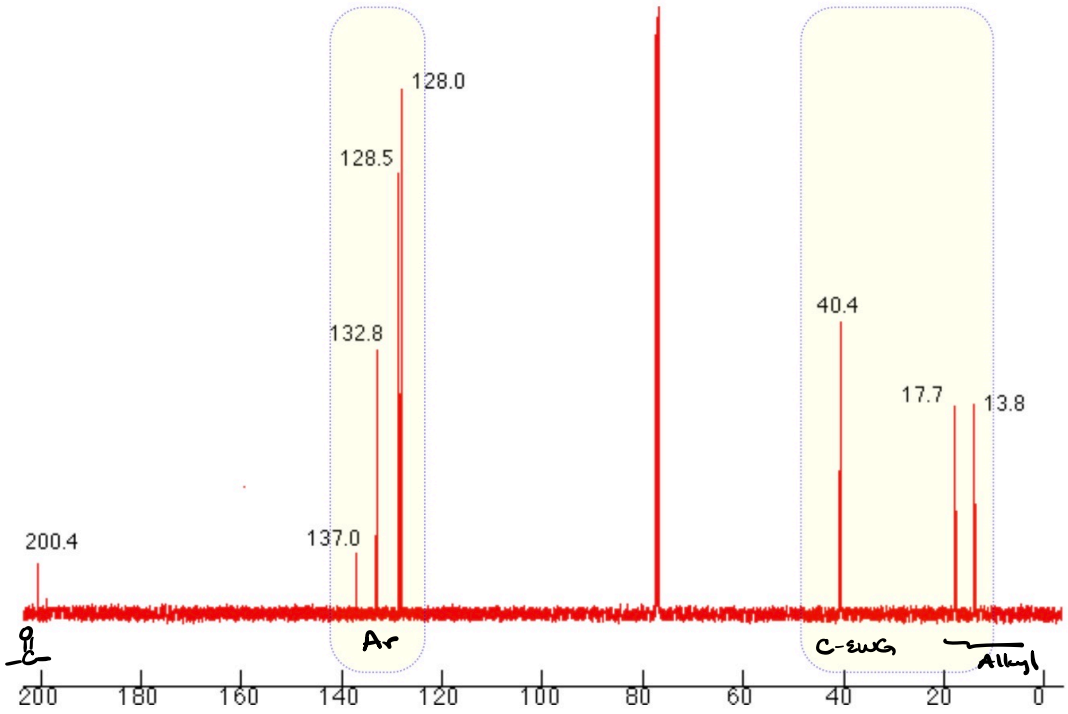
4 units unsat

$C_{10}H_{12}O$

C O 1 unit of unsat

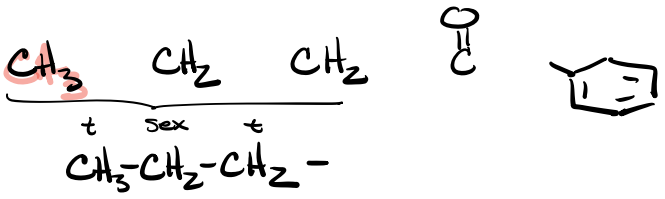


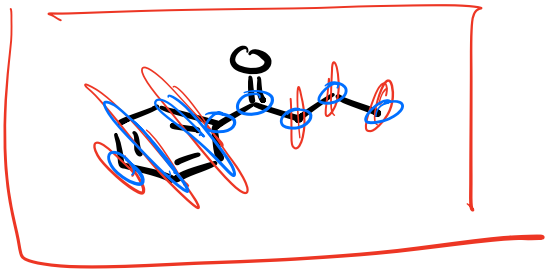
≥ 150



environments = 8

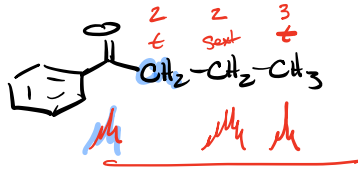
ppm	Assignment
15	Alkyl
20	
40	
128.0	Ar
128.5	
132	
137	
200	C=O

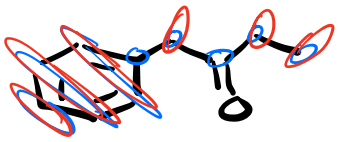




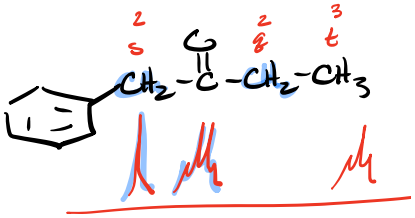
H C mult

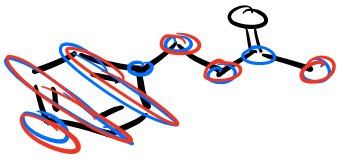
6 8



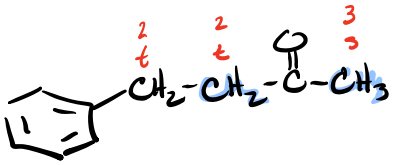


6 8



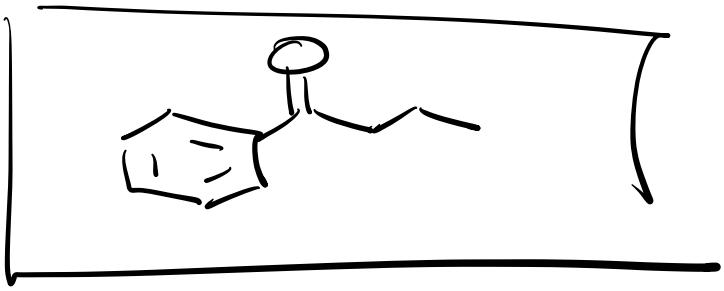


6 8



No methyl CH_3

No 12.0 in HNMR 



19 $C_9H_7NO_4$

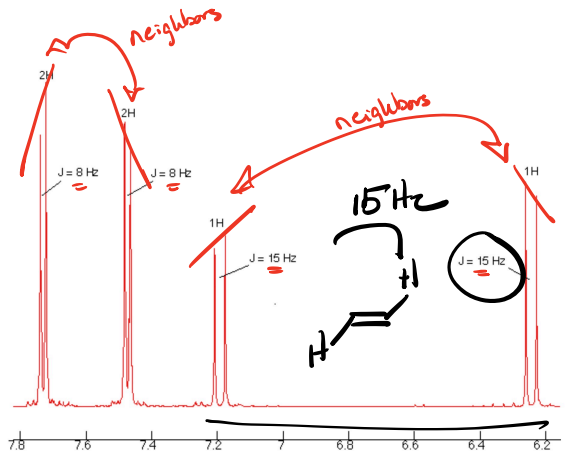
$C_nH_{2n+2+N-X}$?

for Sat

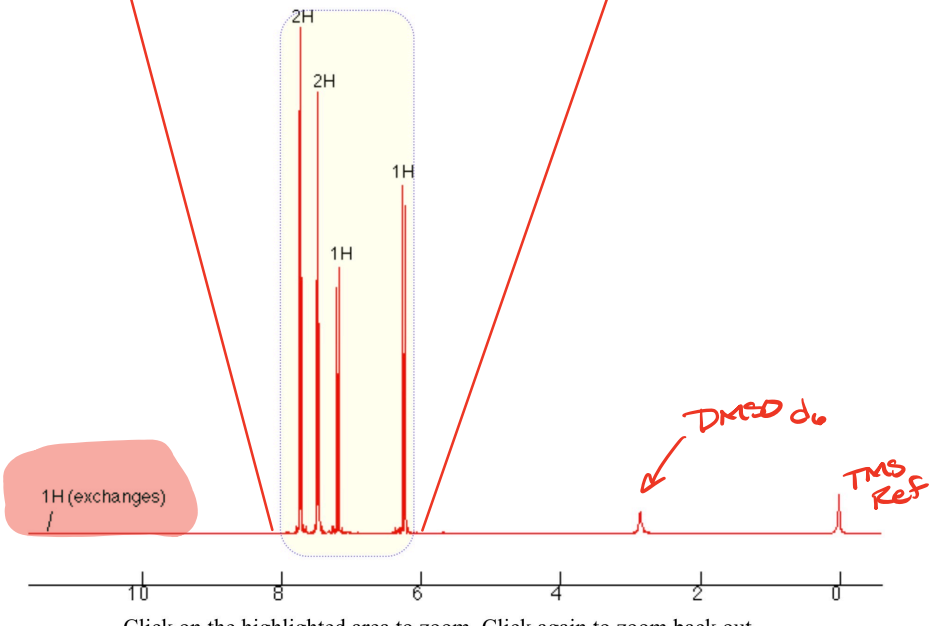
$2(9) + 2 + 1$ ← for N $= 21$

$$\begin{array}{r} 21 \\ -\ 7 \\ \hline 2\,|\,14 \end{array}$$

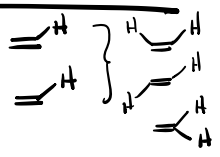
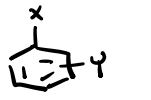
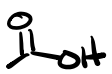
7 units unsaturation ⇒ Aromatic + 3 more units



Problem 19 - ^{1}H NMR spectrum (DMSO-d_6, 300 MHz)



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

ppm	Int	mult	# neighbors	Assignment
6.2	1	d	1 (15Hz)	
7.2	1	d	1	
7.45	2	d	1 (8Hz)	Ar 
7.65	2	d	1	
11.2	1	s	∅	Exchanges –OH 

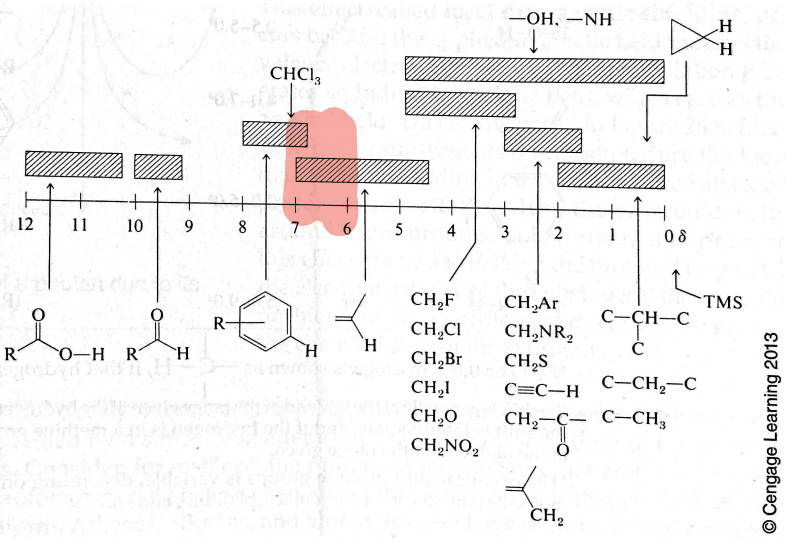
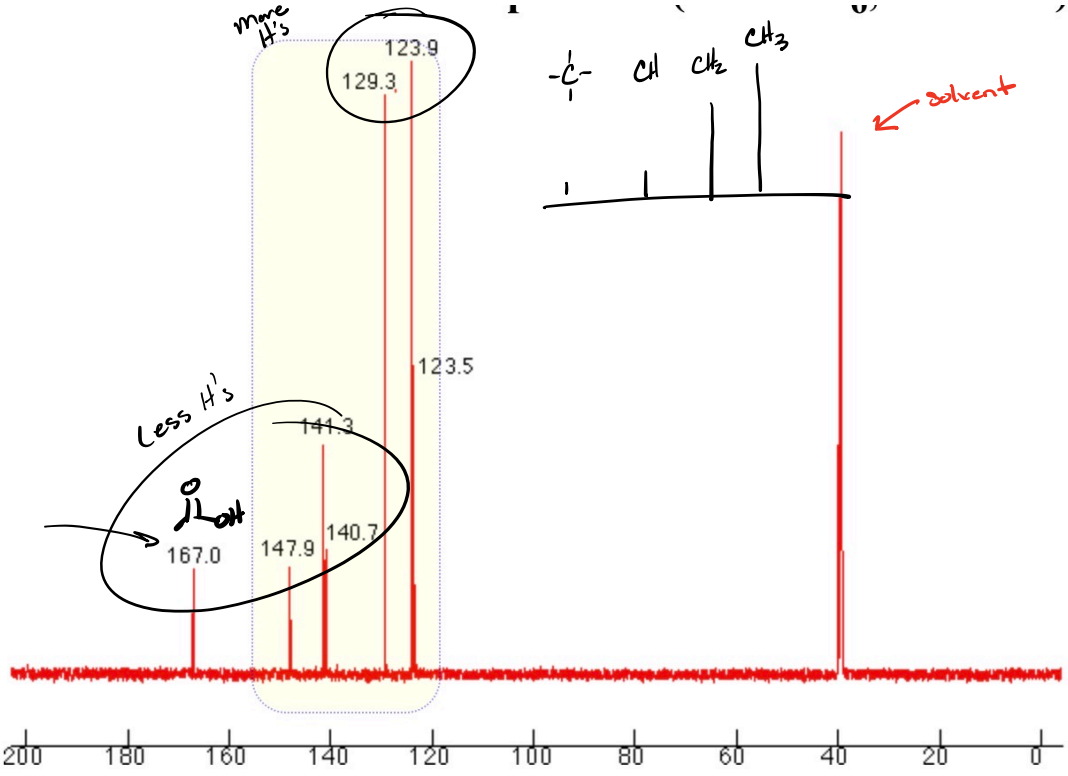
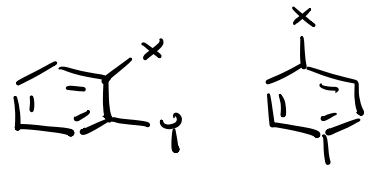


Figure 26.7
A simplified correlation chart for proton chemical shift values.



Chemical Environments = 7

ppm	Assignment
123.5	Alkene =
123.9	
129.3	Ar
140.7	
141.3	
147.9	
167.0	



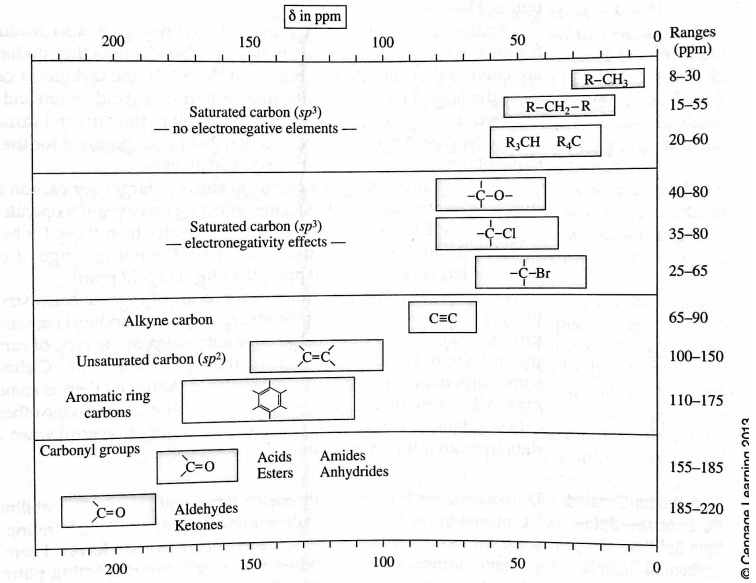
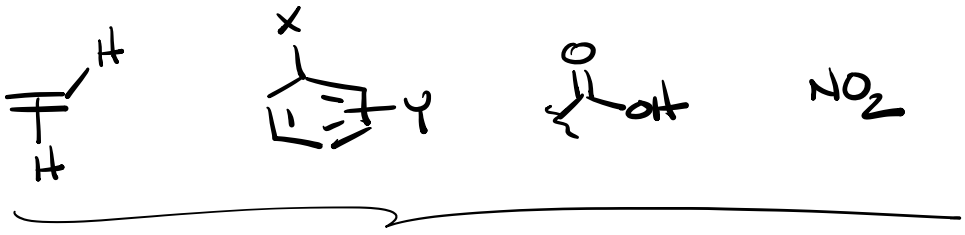


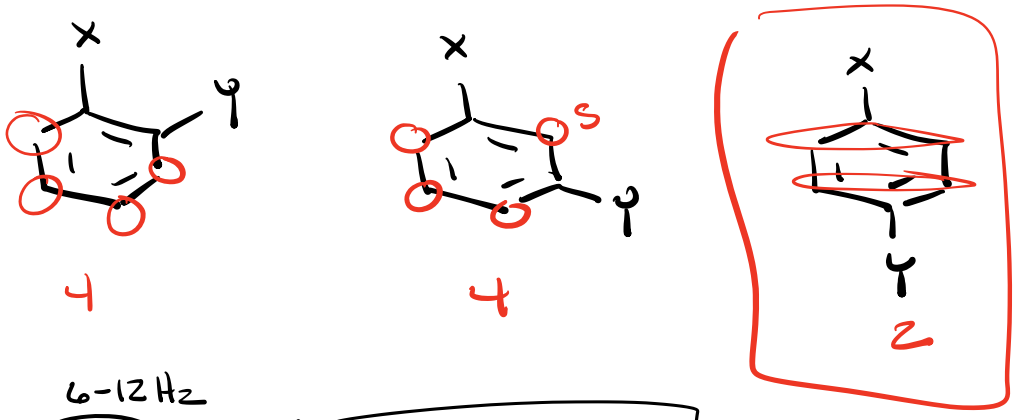
Figure 27.1
A correlation chart for ^{13}C chemical shifts (chemical shifts are listed in parts per million from tetramethylsilane).

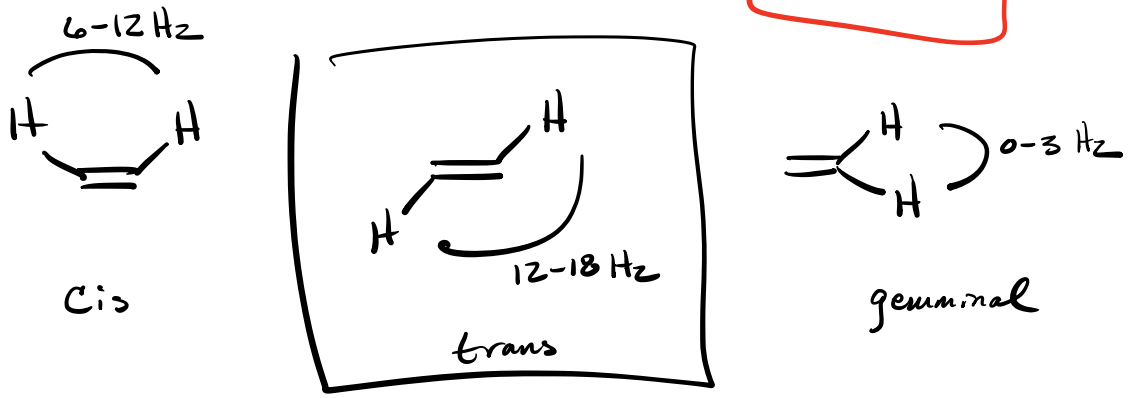


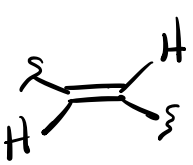
$C_9H_7NO_4$ ✓

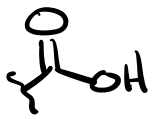
decide Ring

Double bond ✓

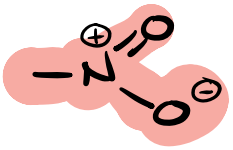




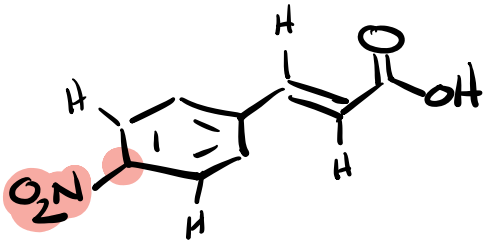


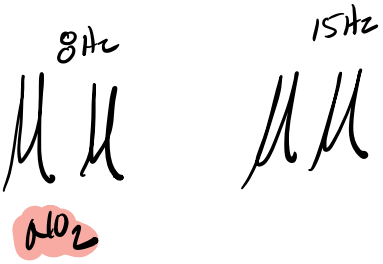


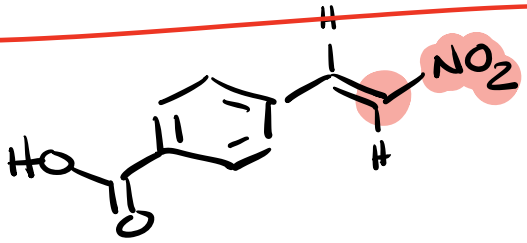
$-NO_2$

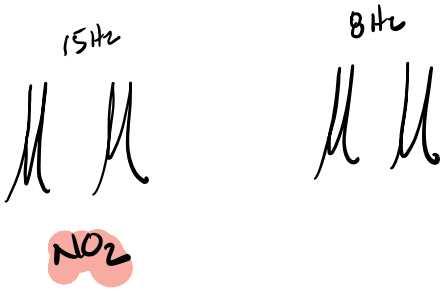


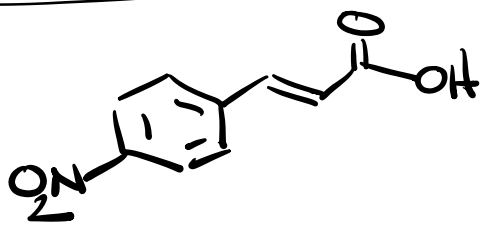
terminal











Check formula
Check Chemical Env.
Check HNMR
Spl. Hing & Int