NMR #3, 6, 7, 8 on Webspectra

#3 $C_4H_7O_2Br$

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

$2(4)+2-1 = 9$

9 sat
-7 Given
2 | 2
1 unit unsat

---

1 ring
C=C
C=O ⟹ 

Procedure

① units of unsat

② ^{1}H-NMR & ^{13}C-NMR
1st Impressions

③ Deep dive into ^{1}H-NMR
Table of data

④ Same for Carbon

⑤ Look to see are they saying same thing?

⑥ Look for or identify parts

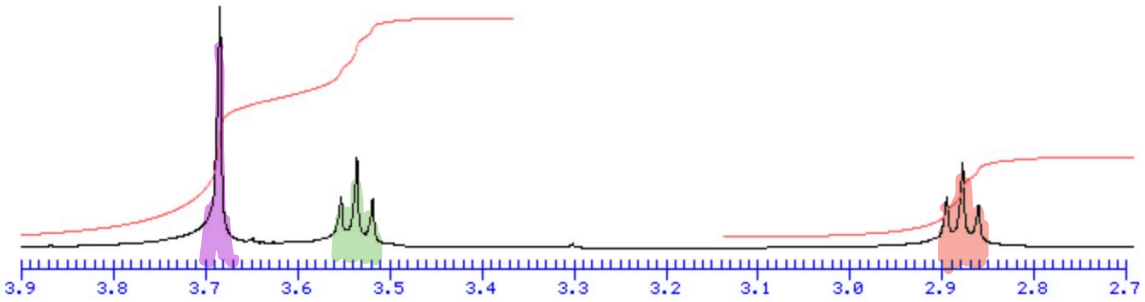
⑦ Look for connectivity

⑧ Look back at units of unsat

⑨ Start drawing options

⑩ Start eliminating options

⑪ Eliminate until down to 1



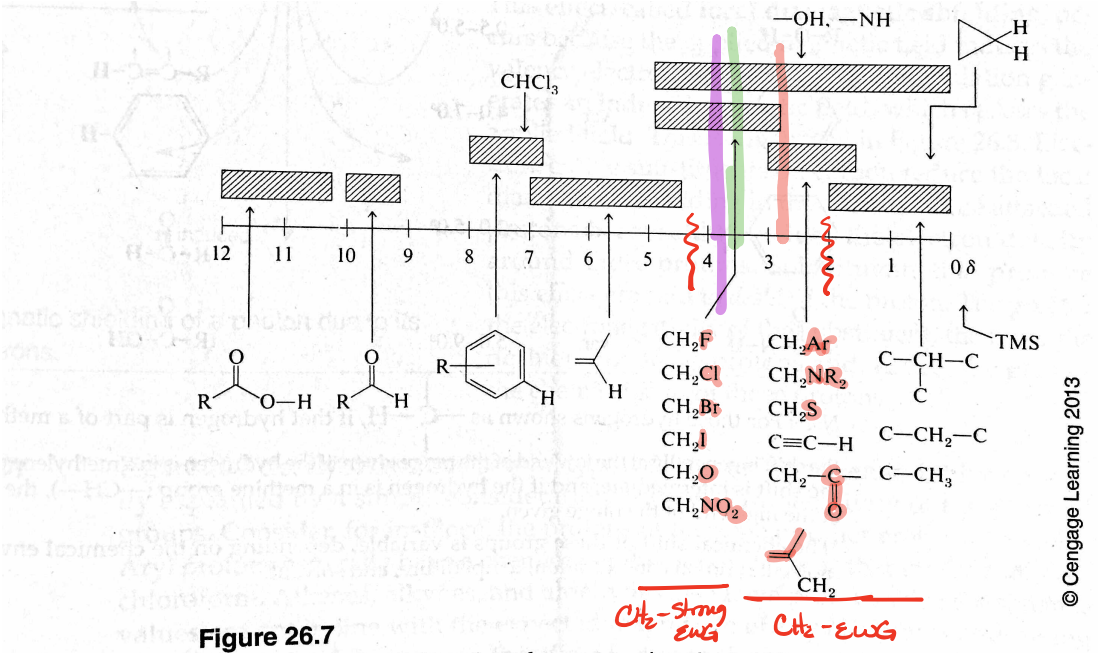


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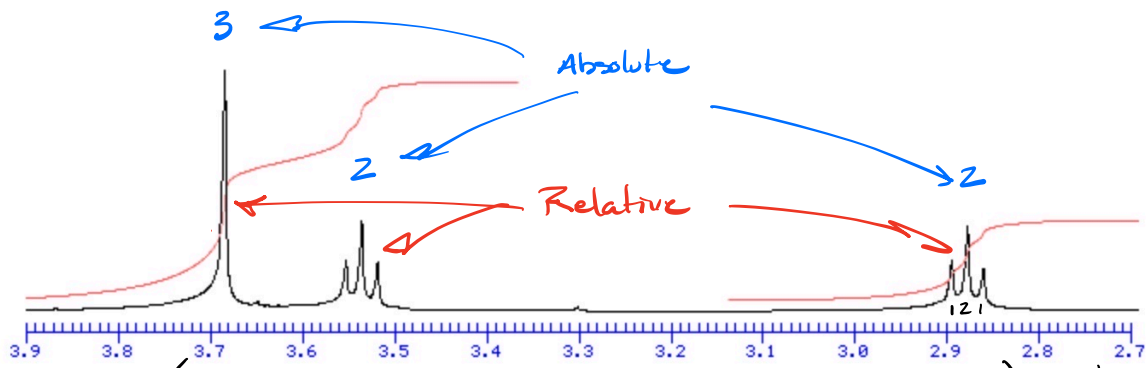
Figure 26.7
A simplified correlation chart for proton chemical shift values.



2 (2 / 4 3) 1 / 2) 1 = 4 = 8 = 7

¹HNMR # of environments 3

δ ppm	Int	multiplicity	# neighbors	Assignment
2.89	2	3	2	CH_2-CH_2-EWG (X = $C(H)-CH_2-EWG$, 5 bonds to Carbon)
3.55	2	3	2	CH_2-CH_2-EWG (neighbors)
3.7	3	1	∅	CH_3 – strong EWG, Isolated

Parts

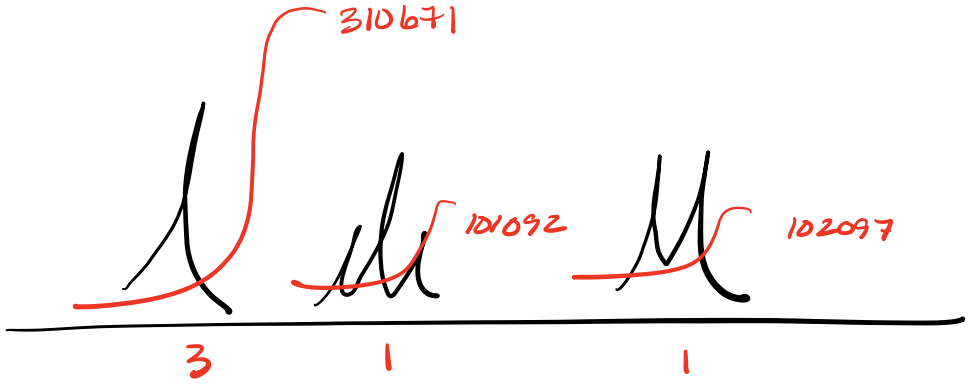
CH_3 – Strong EWG (3)

$^2EWG-CH_2-CH_2-EWG^1$

C_3H_7

Missing
Br
20
C ✓

Integrations are always Relative



$\frac{310671}{102097} \approx 3$ $\frac{101092}{102097} \approx 1$ $\frac{102097}{102097} = 1$

$3 : 1 : 1$

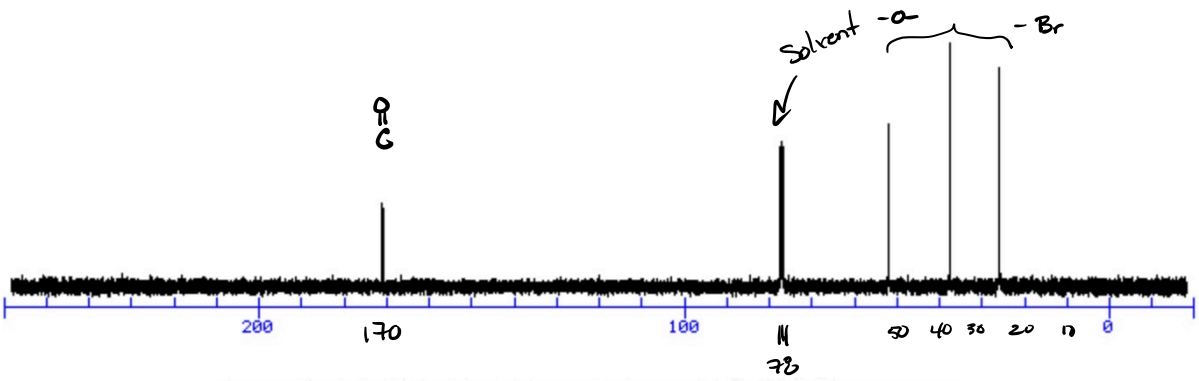
$\times 2 \rightarrow 6 : 2 : 2$

$\times 3 \rightarrow 9 : 4 : 4$

$\times 4 \rightarrow 12 : 6 : 6$

$4 \times 1.25 \quad 1.0 \quad 2$

$5 \quad 4 \quad 8$



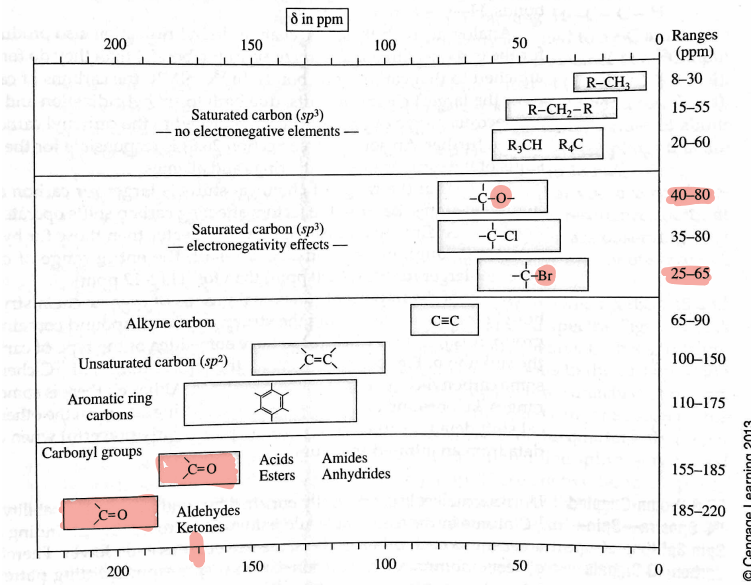


Figure 27.1
A correlation chart for ^{13}C chemical shifts (chemical shifts are listed in parts per million from tetramethylsilane).

$C_4H_7O_2Br$

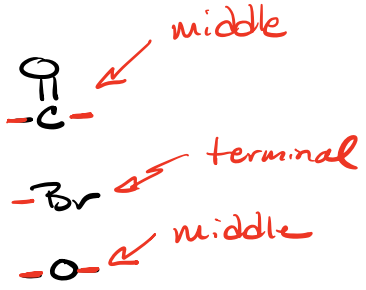
^{13}CNMR Chemical environments = 4

PPM	Assignment
27	C-EWG -Br
39	C-EWG
52	C-EWG -O-
172	C=O

Pieces

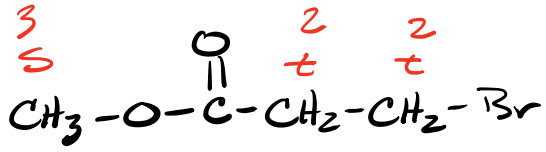
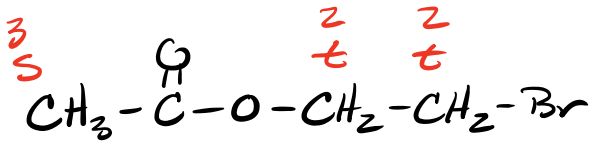
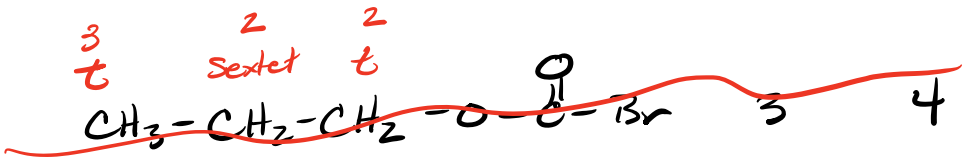
CH_3 - strong EWG

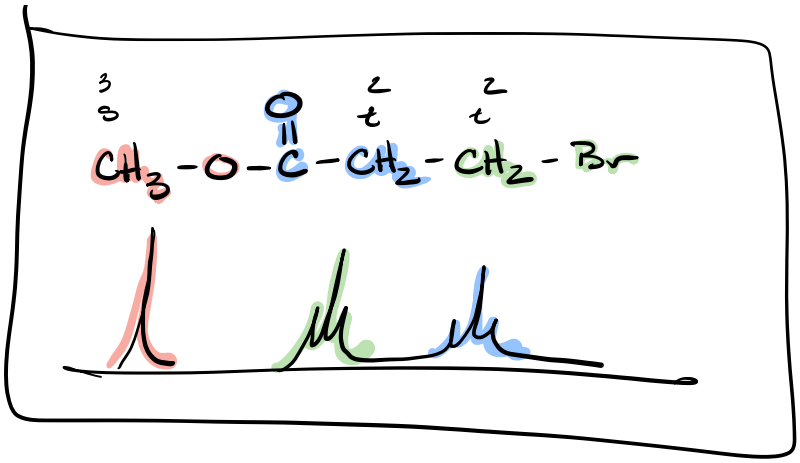
EWG – CH_2–CH_2 – EWG



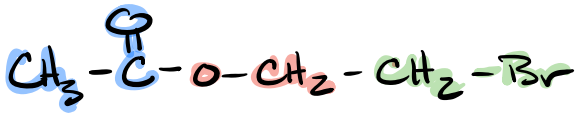
$-CH_2-CH_2-Br$ ~~CH_3-Br~~

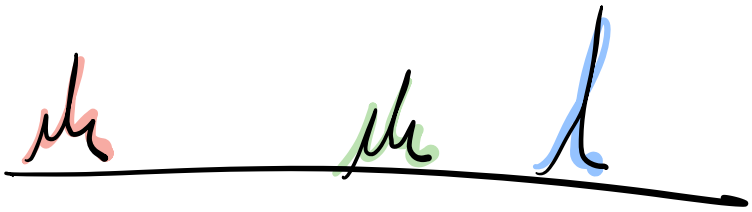
Splitting

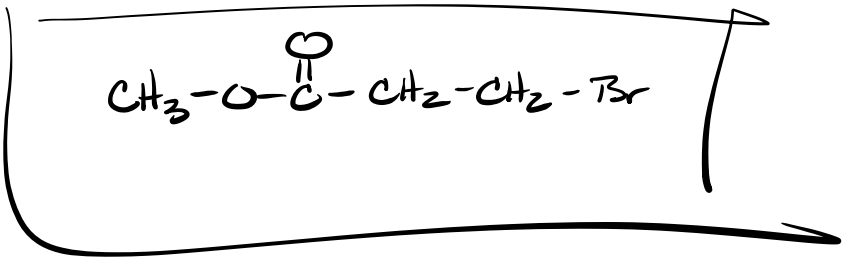
	^1H	^{13}C
	3	4
	3	4
	3	4



match



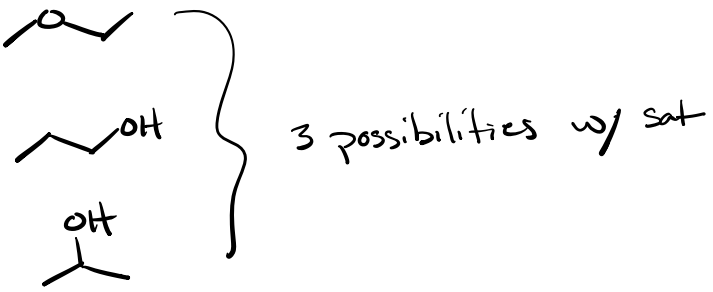




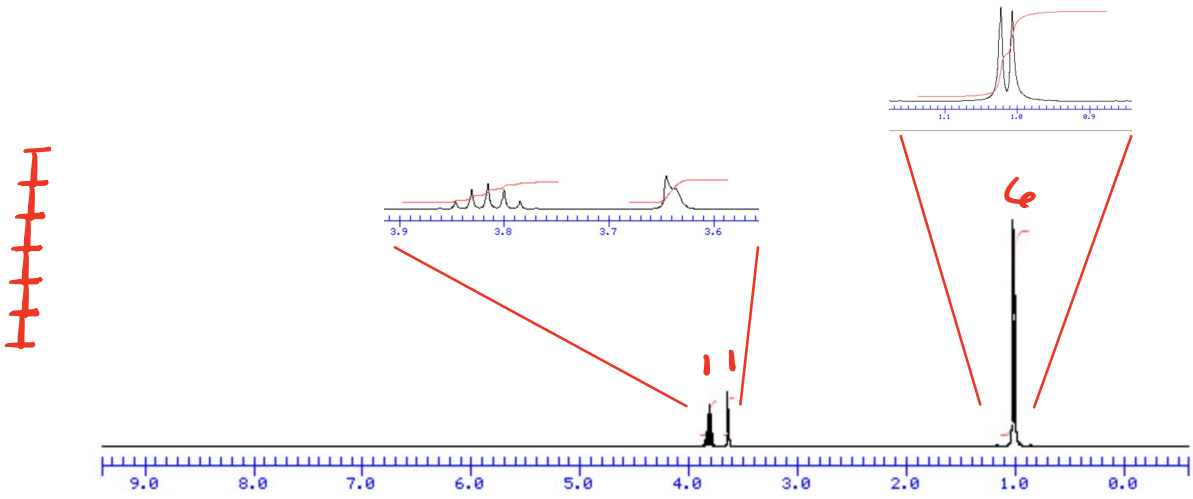
#6 webspectra

C_3H_8O Saturated

$2(3)+2 = 8$

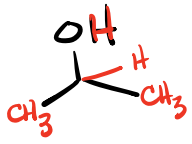


^{1}HNMR

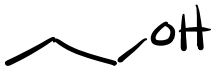


environments

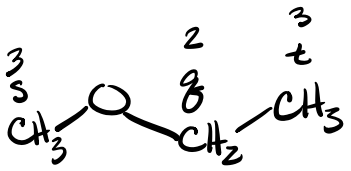

3

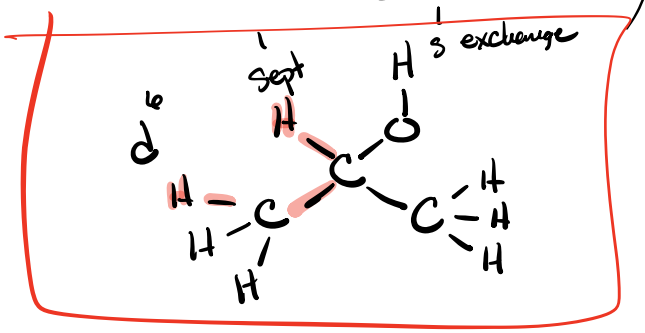


3



4





1 : 5 : 10 : 10 : 5 : 1

3 t 2 sext 2 t — 1's exchanges

$CH_3-CH_2-CH_2-O-H$

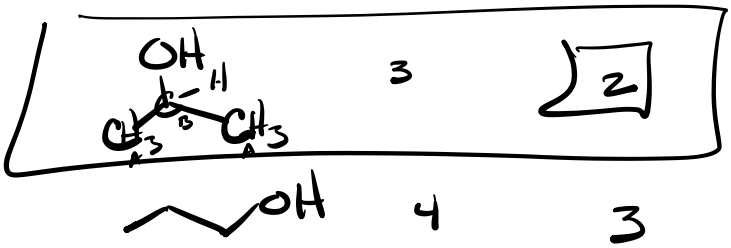
tq 2

multiplet

1
1 1
1 2 1
1 3 3 1
1 4 6 4 1
1 5 10 10 5 1

2 — exchanges — 1 — 2 — 3

H / 3 — C / 3



4 — 3

#7 Web Spectra

$C_{14}H_{14}$

$2(14)+2 = 30$

$30 - 14 = 16$

$16 \div 2 = 8$ units unsat

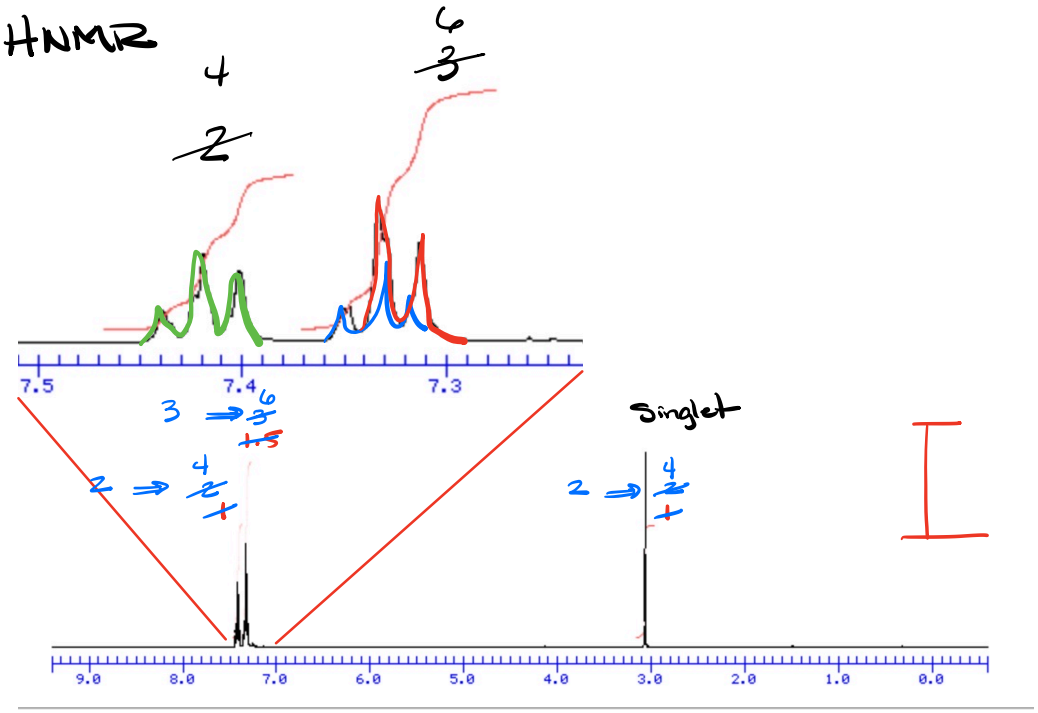
→ Aromatic

 x2

4 units

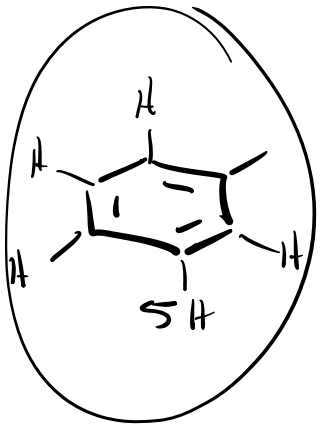
Symmetry

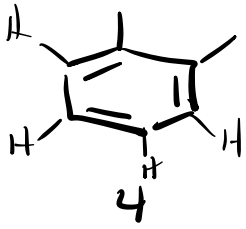
^{1}HNMR

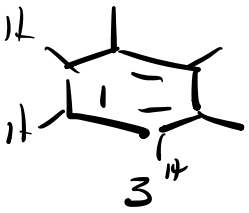


Chemical Environments – 3

ppm	Int	mult	# neighbors	Assignment
3.0	4	s	ø	CH_2-Ar x2
7.35	3	t	2	Ar } 10 H's
7.42	2	t	2	Ar }







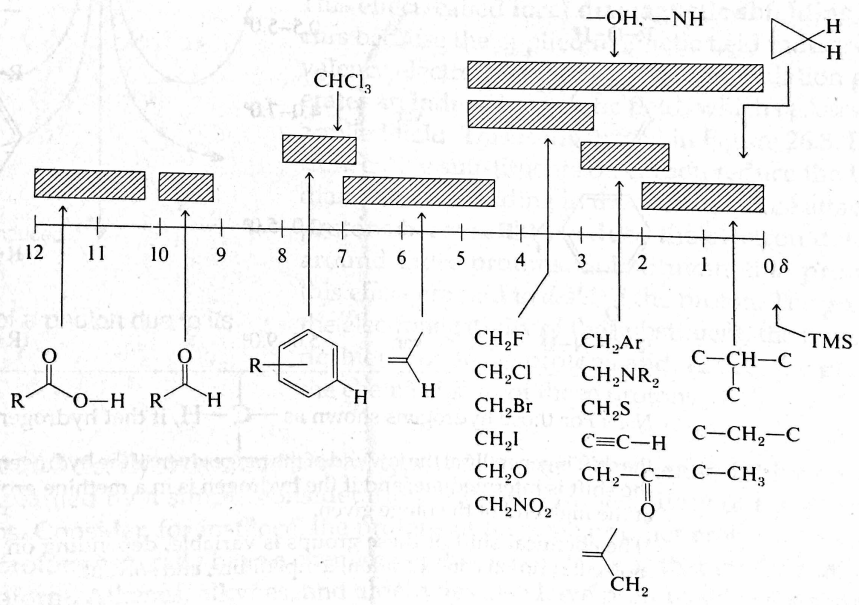


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Figure 26.7
A simplified correlation chart for proton chemical shift values.