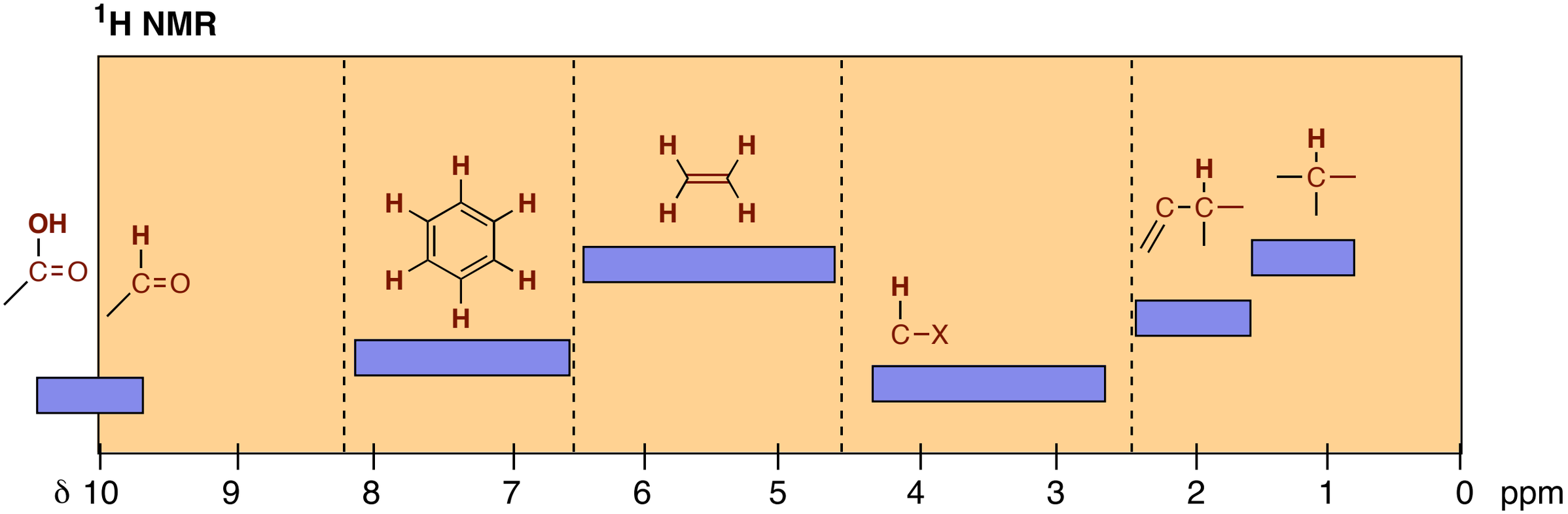
From Last Lecture

- The intensity of the peaks roughly correlates with the number of hydrogens on the carbon.
- DEPT-C13 NMR can tell you exactly how many H's are on the carbons.
- Reactions can be followed by watching functional group changes.
- Symmetry (# of different carbons) is very useful information.
- Proton NMR similar - but more information.

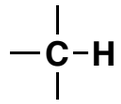
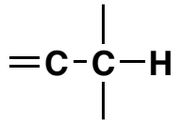
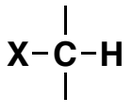
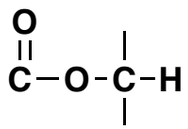
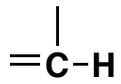
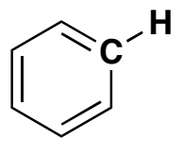
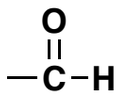
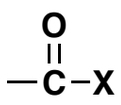
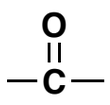
Proton NMR Scale

- Range 0-10 ppm

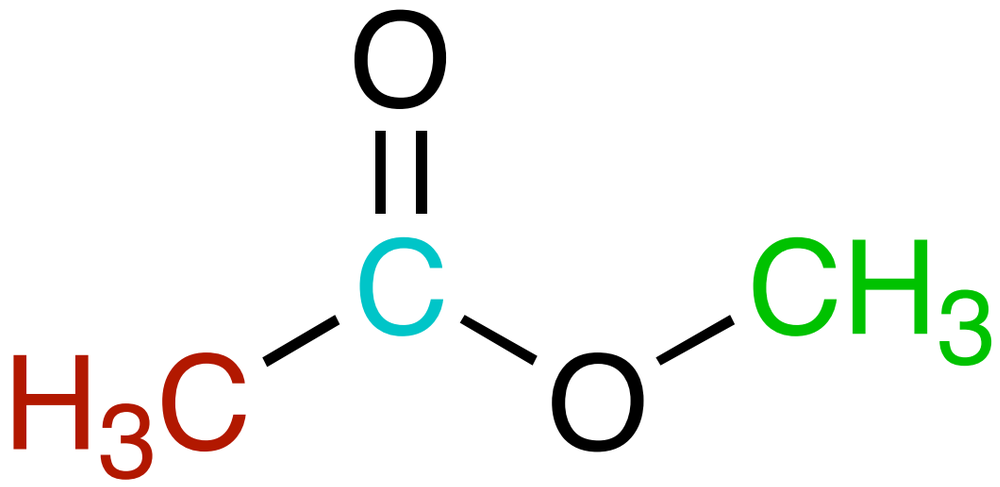


NMR Correlation Chart

Typical NMR Chemical Shifts

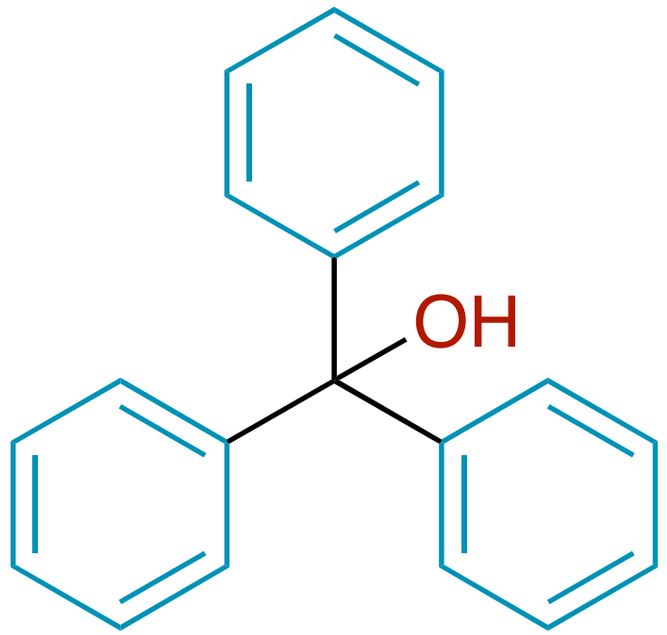
Functional Group	Type	^{1}H Chemical Shift (ppm)	^{13}C Chemical Shift (ppm)
	Alkane	0.7 -1.8	10 - 60
	Allylic or next to carbonyl	1.6 - 2.4	30 - 60
	next to halogen or alcohol	2.5 - 4.0	20 - 85
	next to oxygen of an ester	4.0 - 5.0	50 - 85
	vinylic	4.5 - 6.5	110 - 150
	aromatic	6.5 - 8.0	110 - 140
	aldehyde	9.7 - 10.0	190 - 220
	alcohol	varies widely will exchange with D_2O	N/A
	carbonyl of ester, amide, or carboxylic acid (X = O, N)	N/A	165 - 185
	carbonyl of ketone or aldehyde	N/A	190 - 220

Methyl Acetate

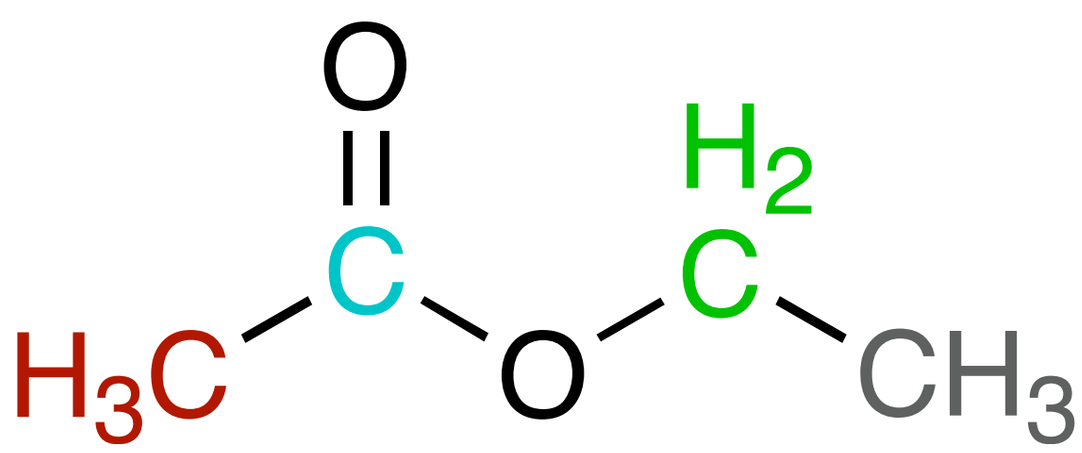


Area under peak corresponds to the number of H's for that resonance

Triphenyl Methanol

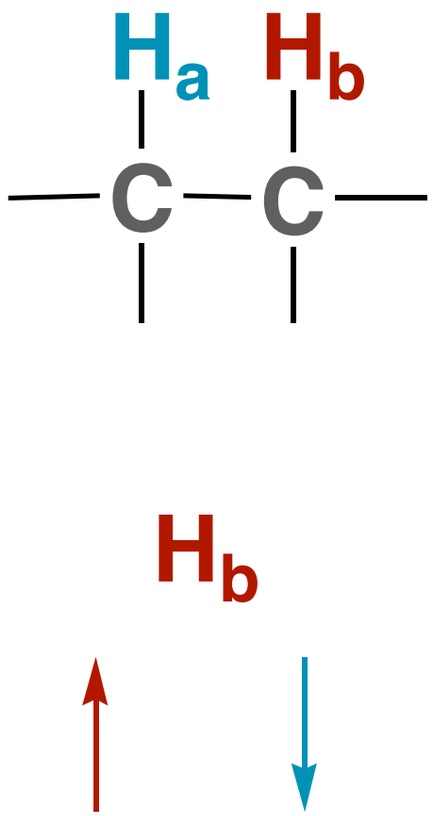


Ethyl Acetate



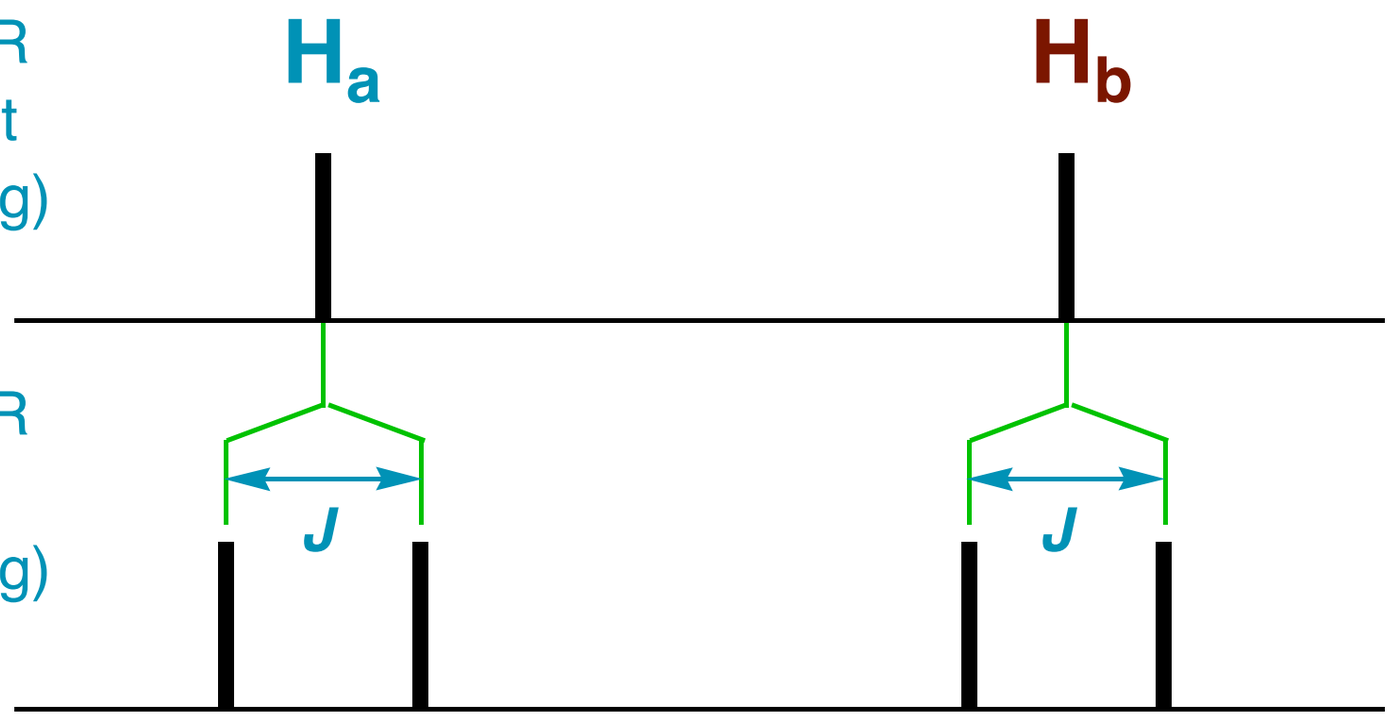
Spin Spin Splitting

- Protons on adjacent carbons also have an effect
- Resonances will split into n+1 number of peaks



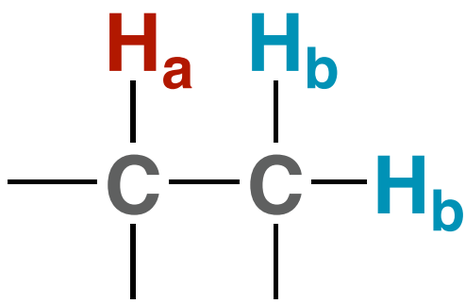
^{1}H NMR (without coupling)

^{1}H NMR (with coupling)

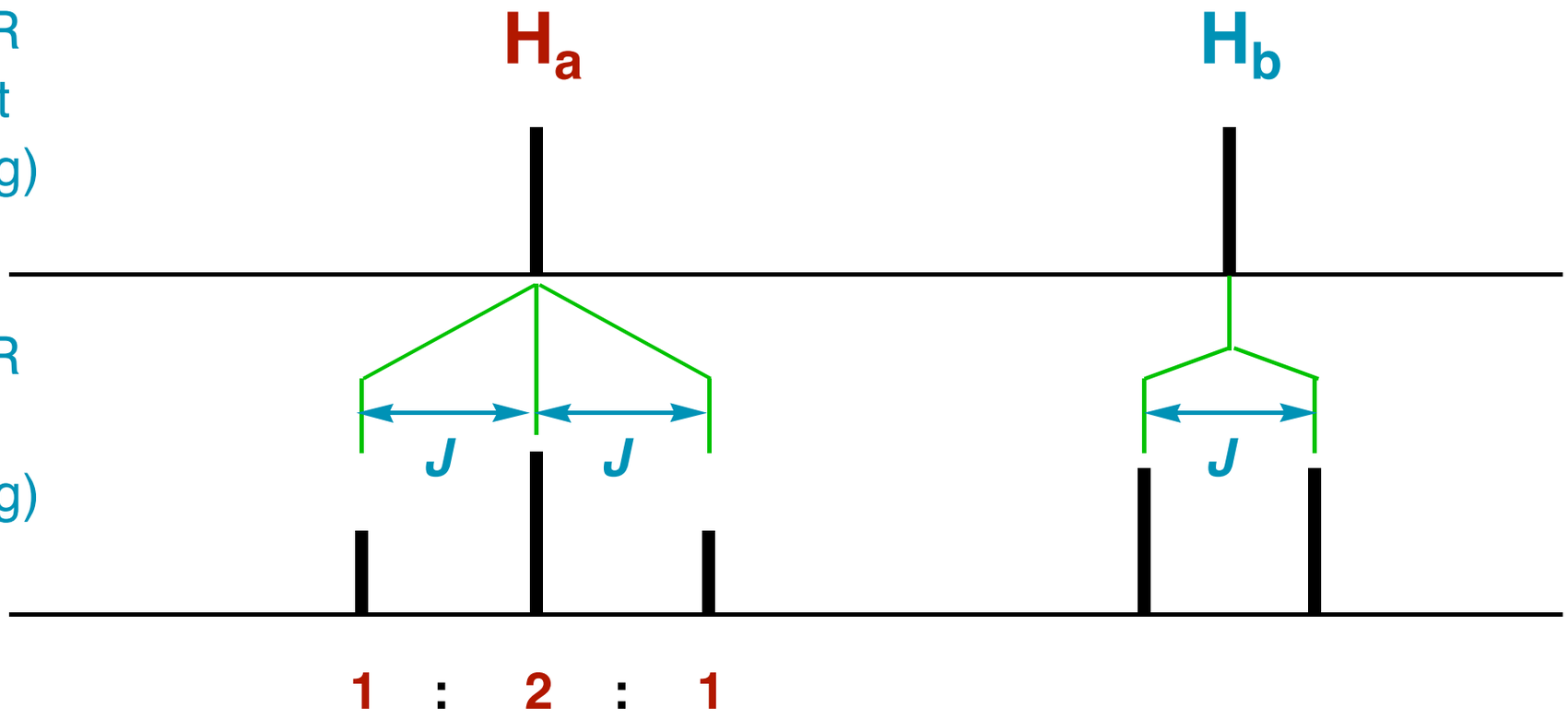


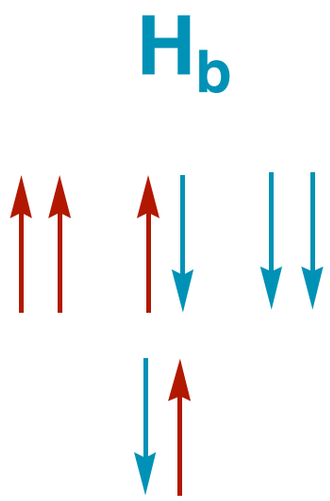
Spin Spin Splitting

- Two hydrogens split neighbors into a triplet



^{1}H NMR (without coupling)

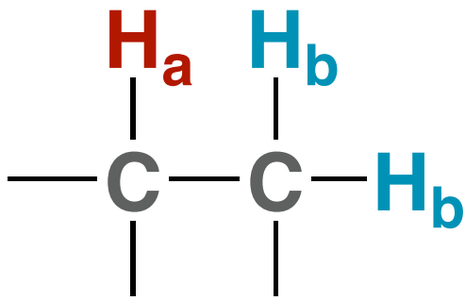


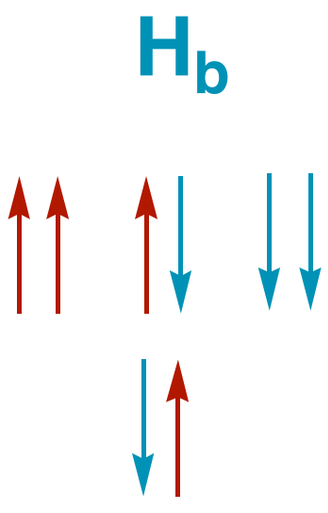


^{1}H NMR (with coupling)

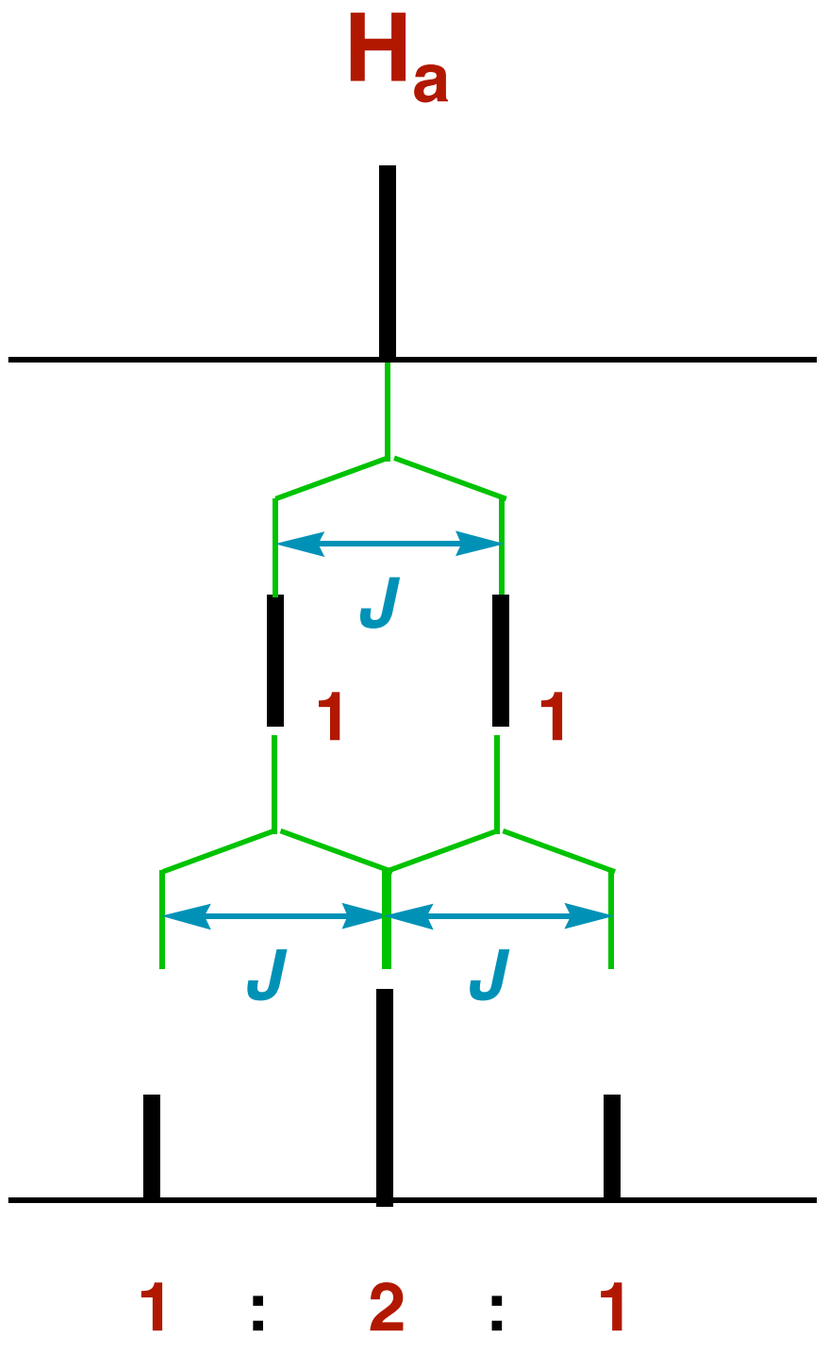
Spin Spin Splitting

- Every splitting can be broken down into a series of doublets



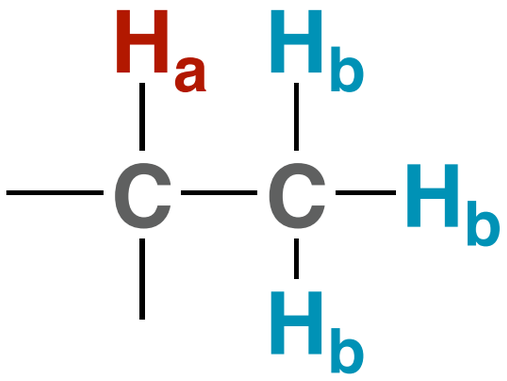


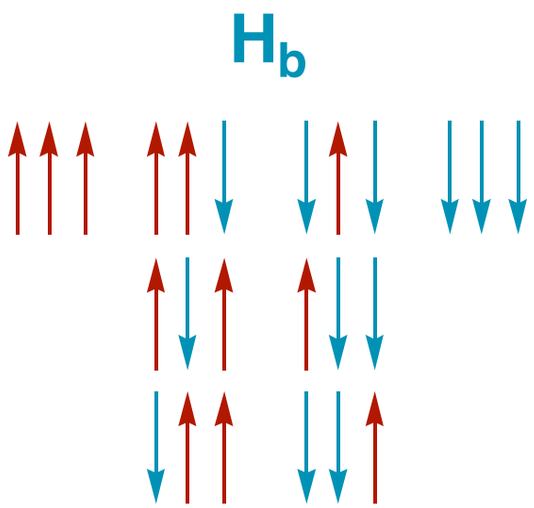
^{1}H NMR (without coupling)

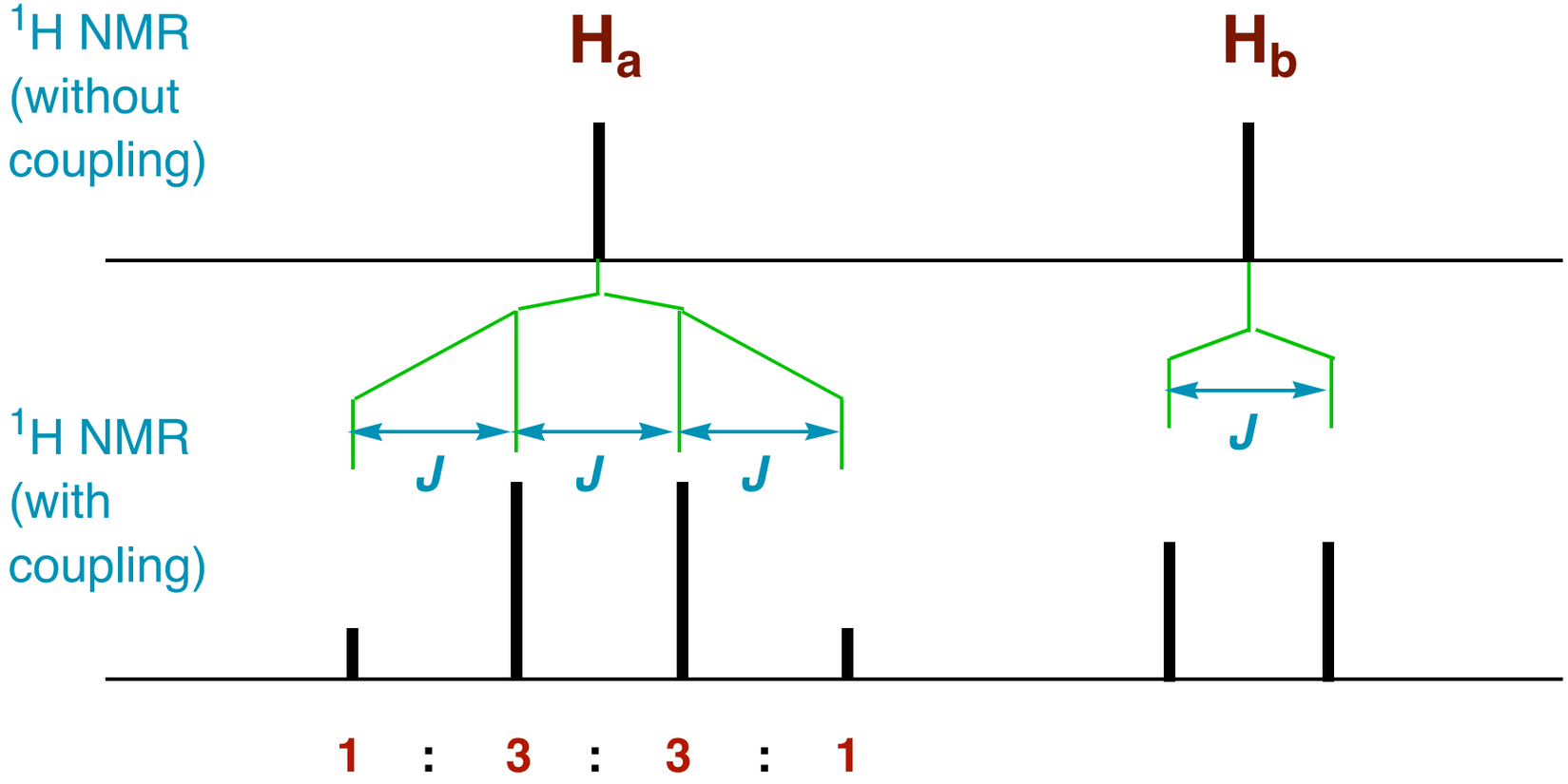


^{1}H NMR (with coupling)

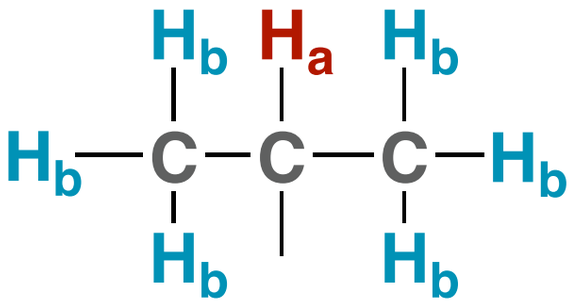
Three neighbors - Quartet







Higher Spin Spin Splitting



H_a will split into 7 peaks

64 different combinations of 6 spins

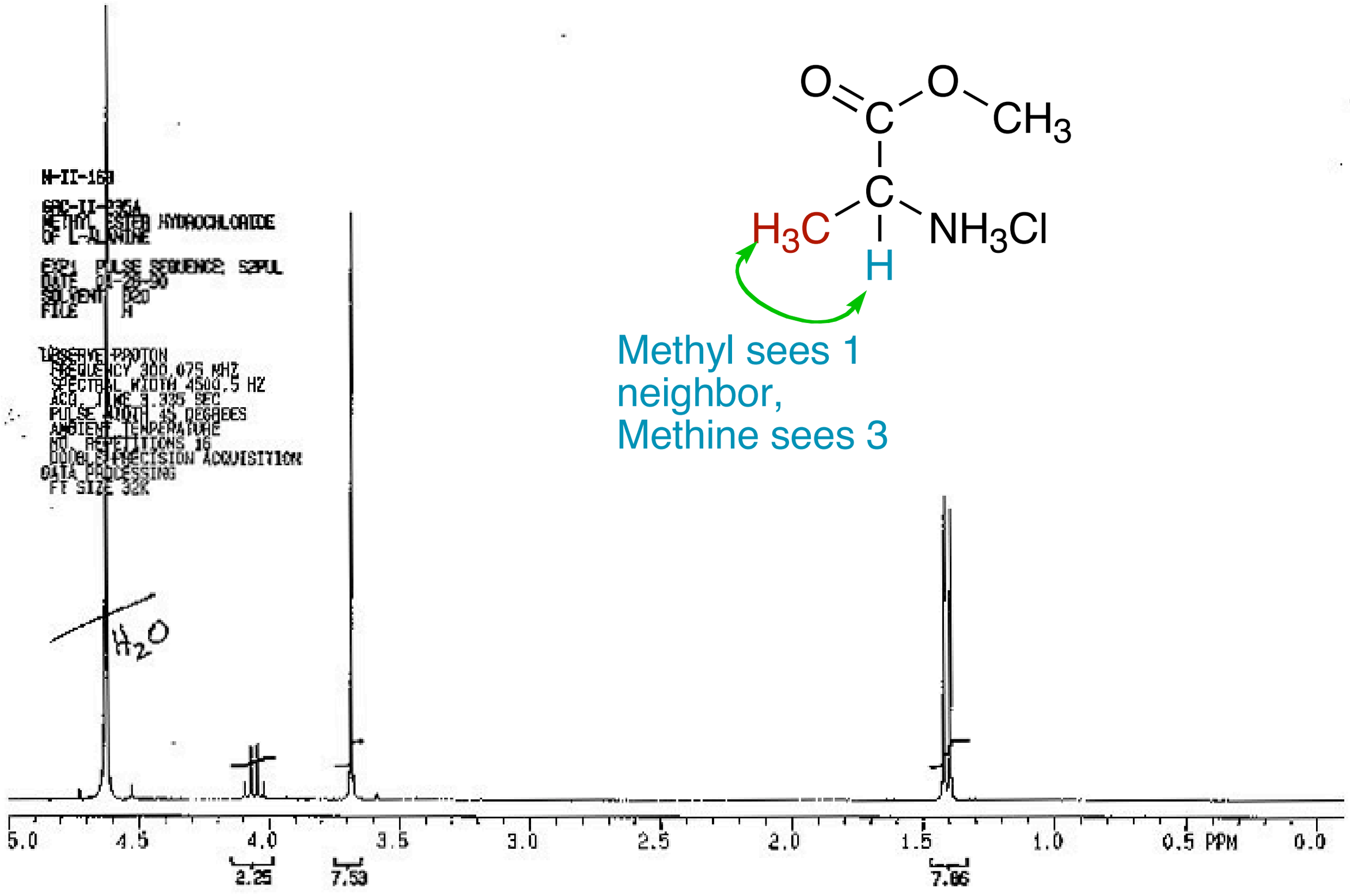
Pascal's Triangle

singlet			1				
doublet		1		1			
triplet			1		2		1
quartet		1		3		3	1
quintet	1		4		6		4		1
sextet		1		5		10		10		5		1
septet	1		6		15		20		15		6		1

Summary of Spin Spin Splitting

- Proton resonance split into n+1 number of peaks
- Relative ratio of peaks depends on number of spin states of the neighbors.
- Adjacent protons will couple with the same coupling constant.
- Protons farther away usually do not couple.
- Chemically equivalent protons cannot couple (eg. $ClCH_2CH_2Cl$).

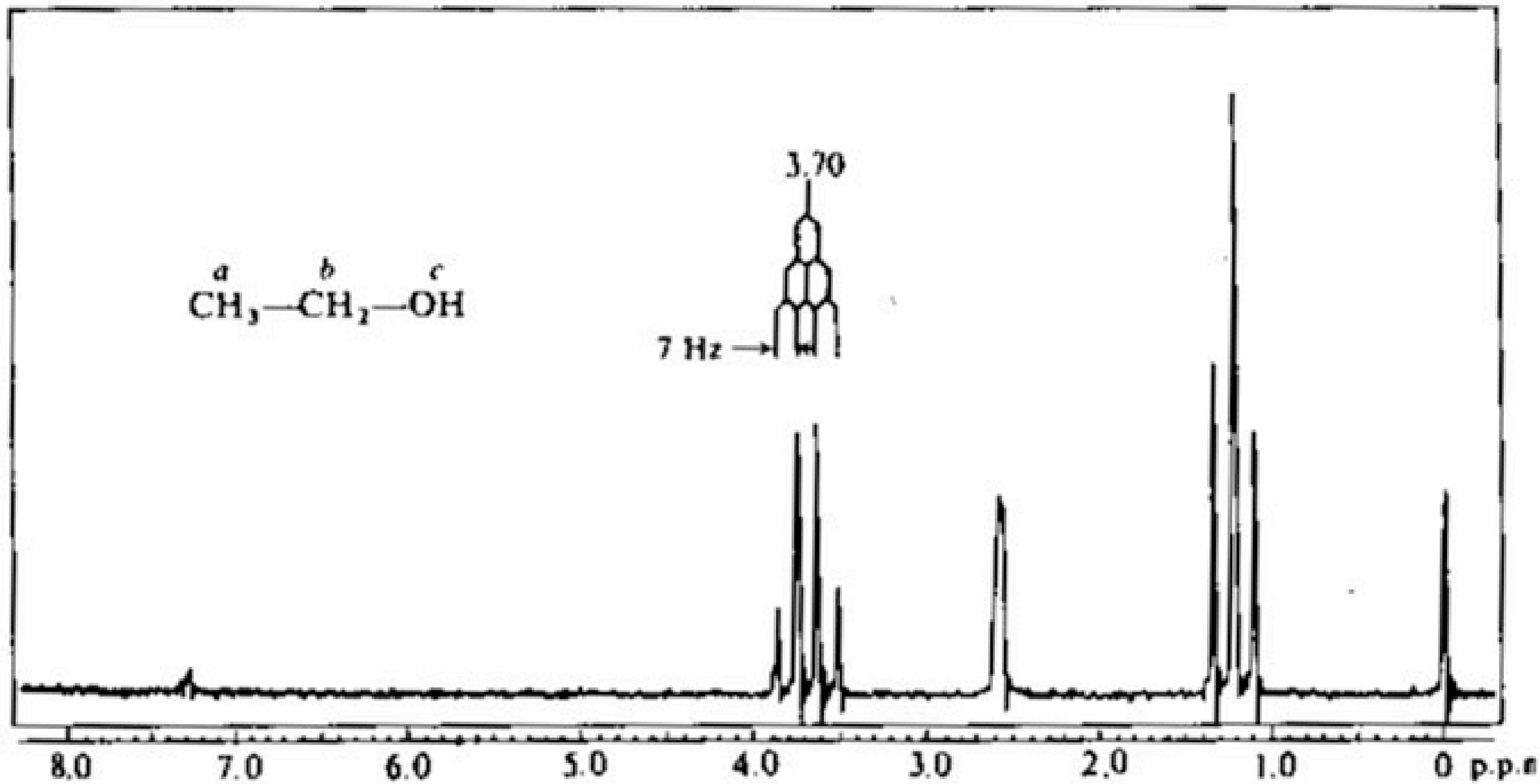
Doublet Splitting



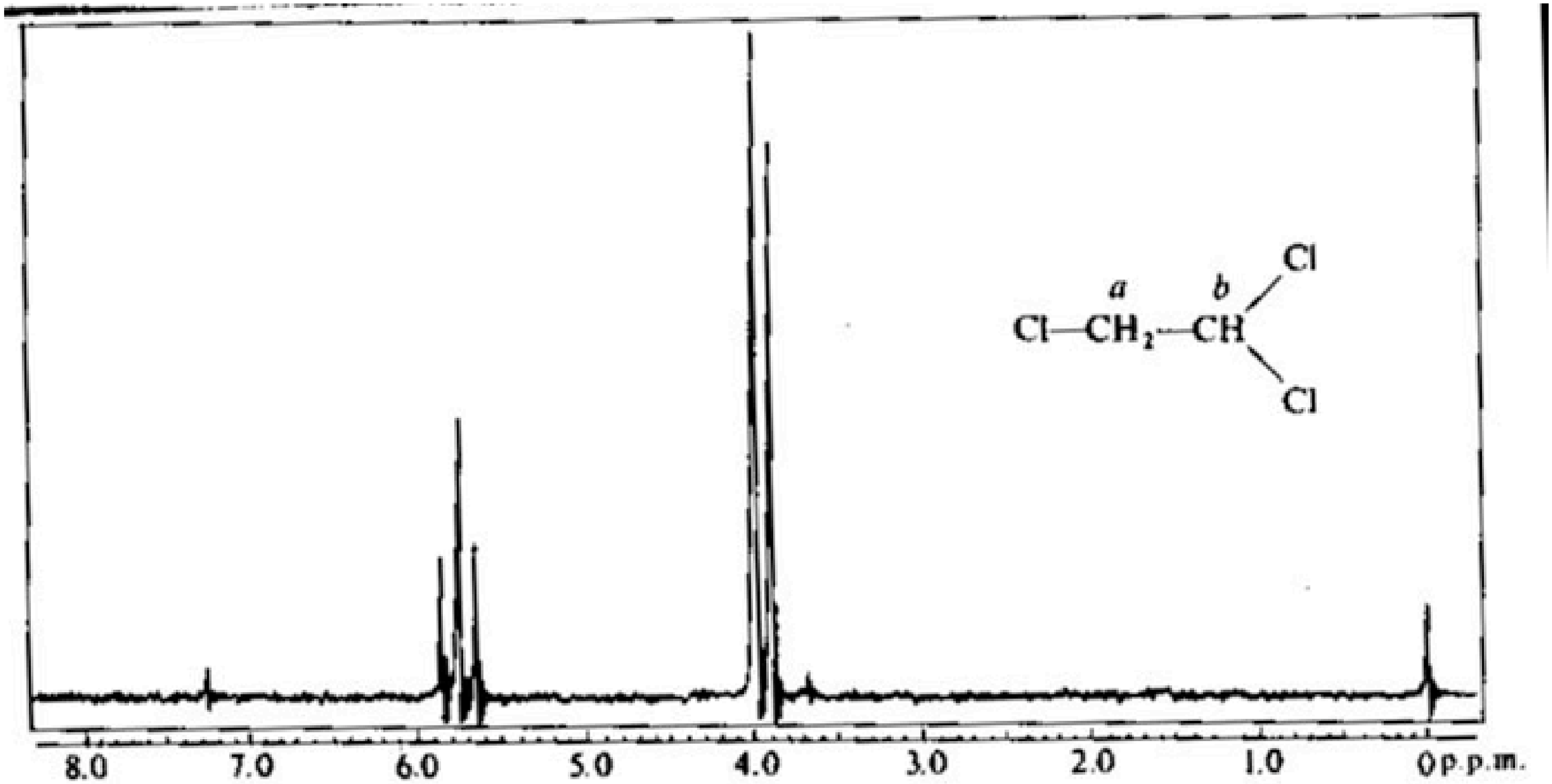
Methyl sees 1 neighbor,
Methine sees 3

Ethanol

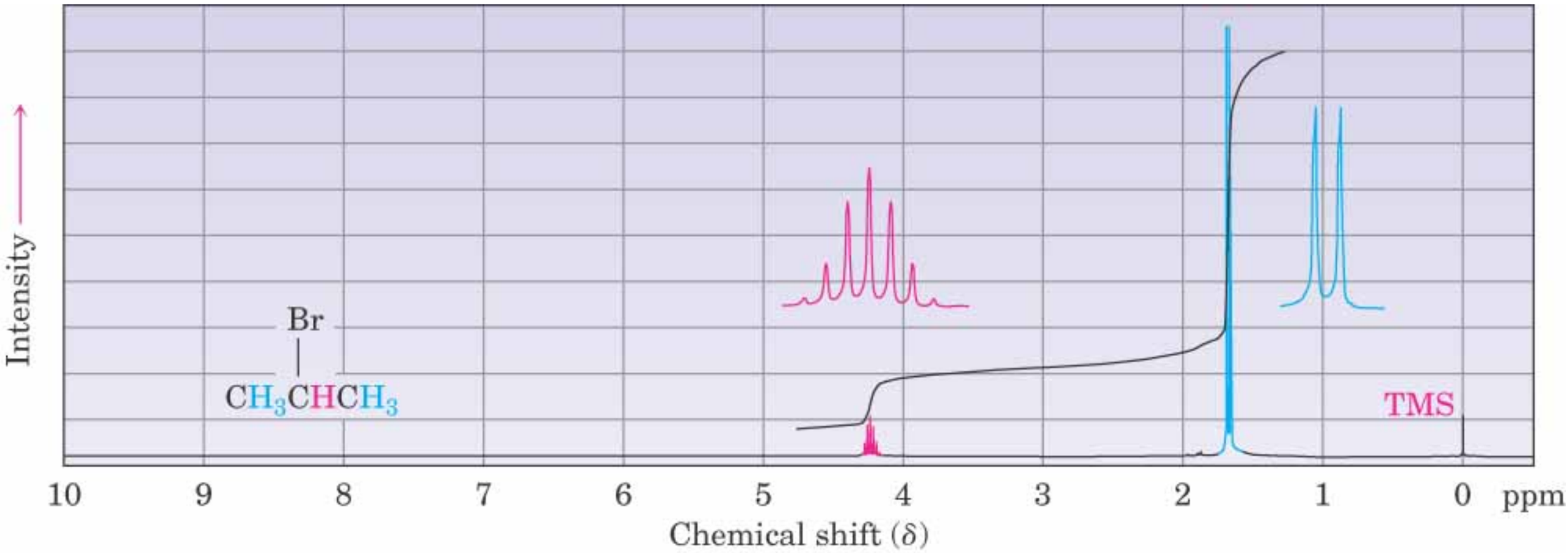
- Note that the OH (and NH) usually don't couple.



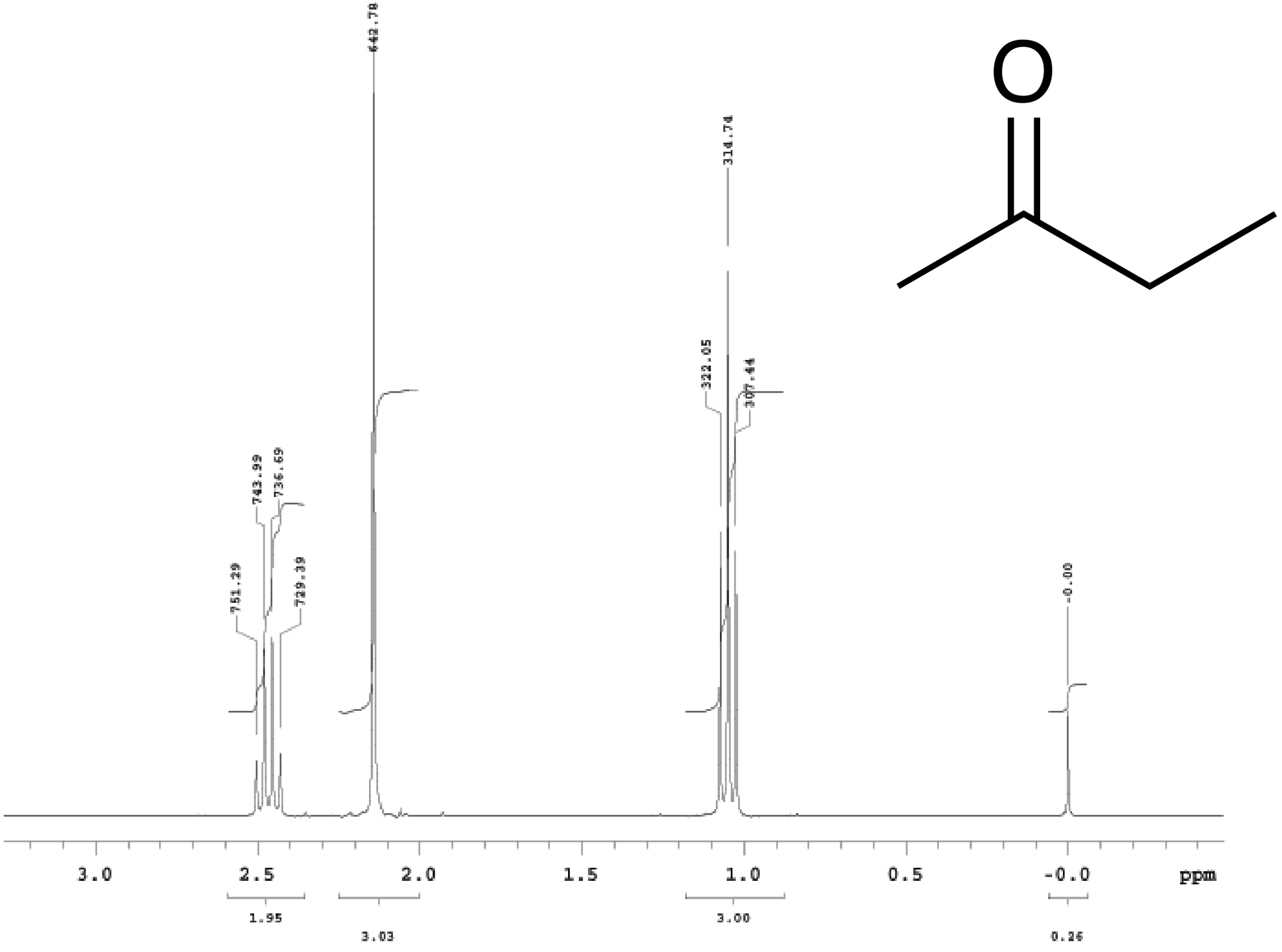
1,1,2-Trichloroethane



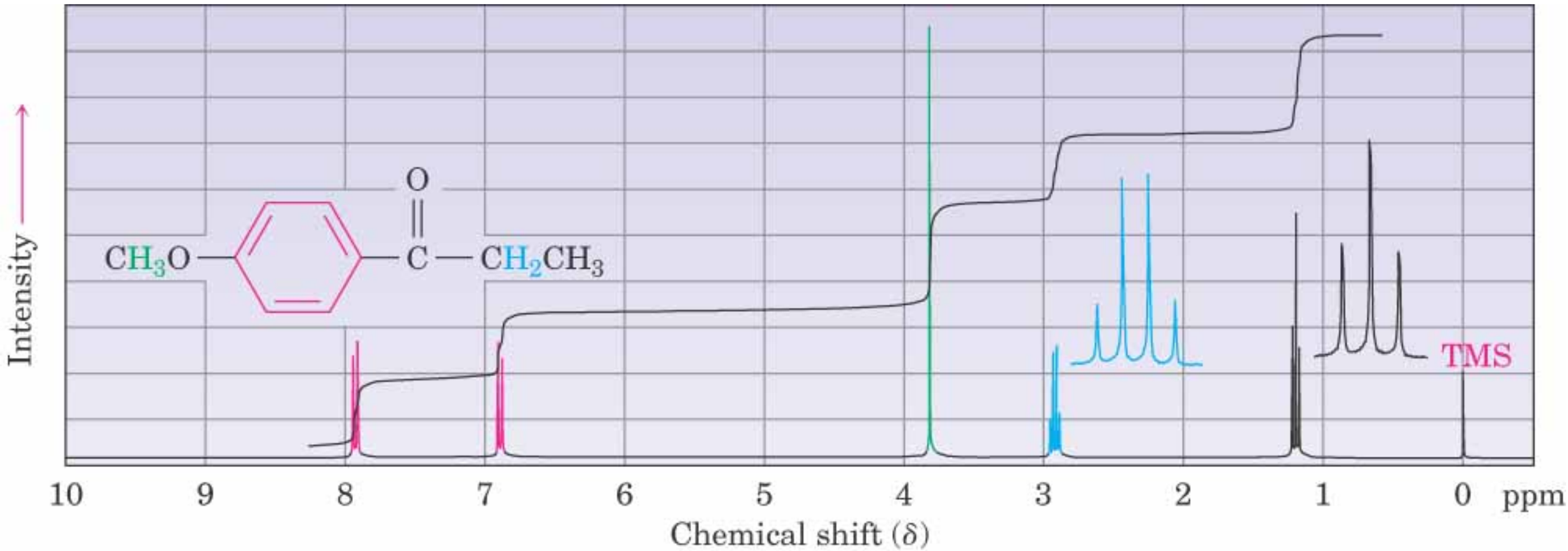
2-Bromopropane



Butanone


642.70
314.74
322.05
307.44
751.29
743.99
736.69
729.39
-0.00
3.0
2.5
2.0
1.5
1.0
0.5
-0.0
ppm
1.95
3.03
3.00
0.26

para-Methoxypropiophenone



Toluene

- Sometimes peaks overlap