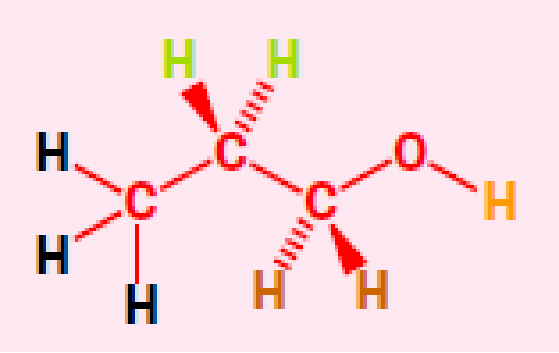
^{1}H-NMR Spectroscopy

^{1}H-NMR Spectroscopy

Except carbon, other major component of the organic molecule is hydrogen atom

Important structural information will be obtain, if we can distinguish between different sorts of hydrogen atoms present

^{1}H nuclei behave similarly as a ^{13}C nuclei does in the magentic field because they have same sipn number I = ½

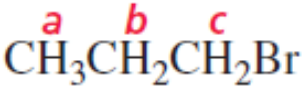


The number of signals in a ^{1}H-NMR spectrum tells you how many different kinds of Hydrogen a compound has—just as the number of signals in an ^{13}C-NMR spectrum tells you how many different kinds of carbon a compound has.

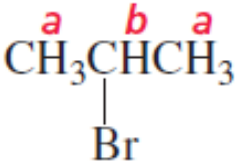
The principles behind ^{1}H-NMR and ^{13}C-NMR spectroscopy are essentially the same.

The Number of Signals in the ^{1}H-NMR Spectrum

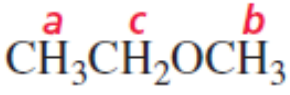
Like carbon**, a set of equivalent protons** gives rise to a signal



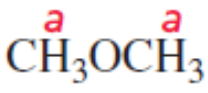
three signals



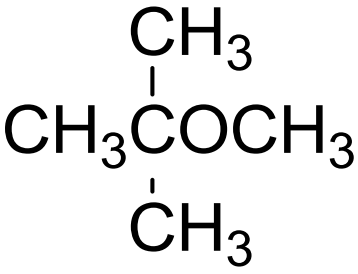
two signals

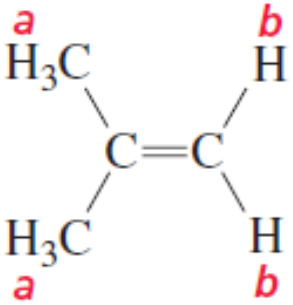


three signals

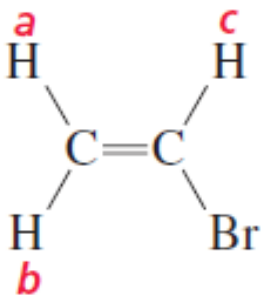


one signal

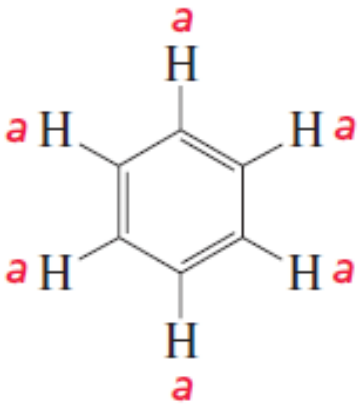




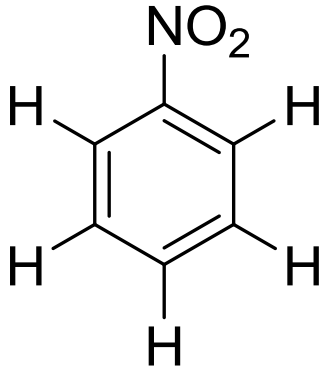
two signals



three signals

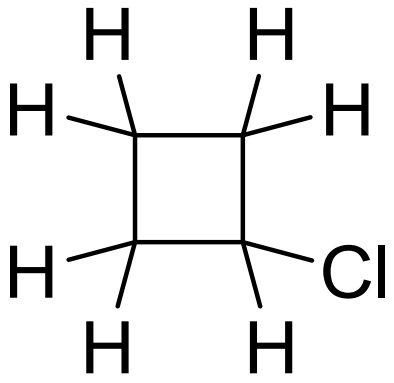


one signal



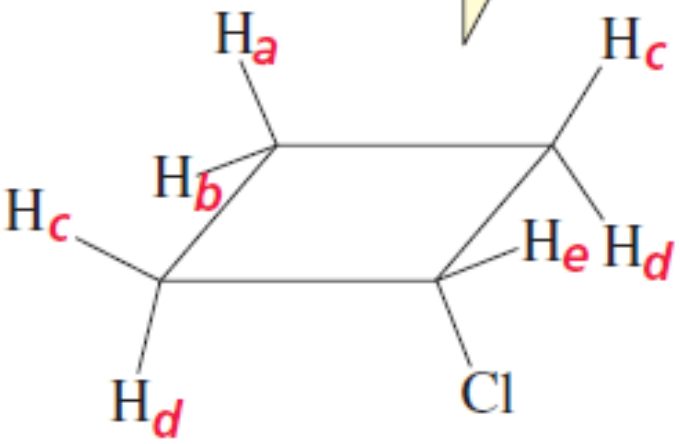
One can tell how many sets of equivalent protons a compound has from the number of signals in its ^{1}H-NMR spectrum

The Number of Signals in the ^{1}H-NMR Spectrum



Sometimes, two protons on the same carbon are not equivalent

its ^{1}H NMR spectrum has five signals



chlorocyclobutane

H_a and H_b are not equivalent

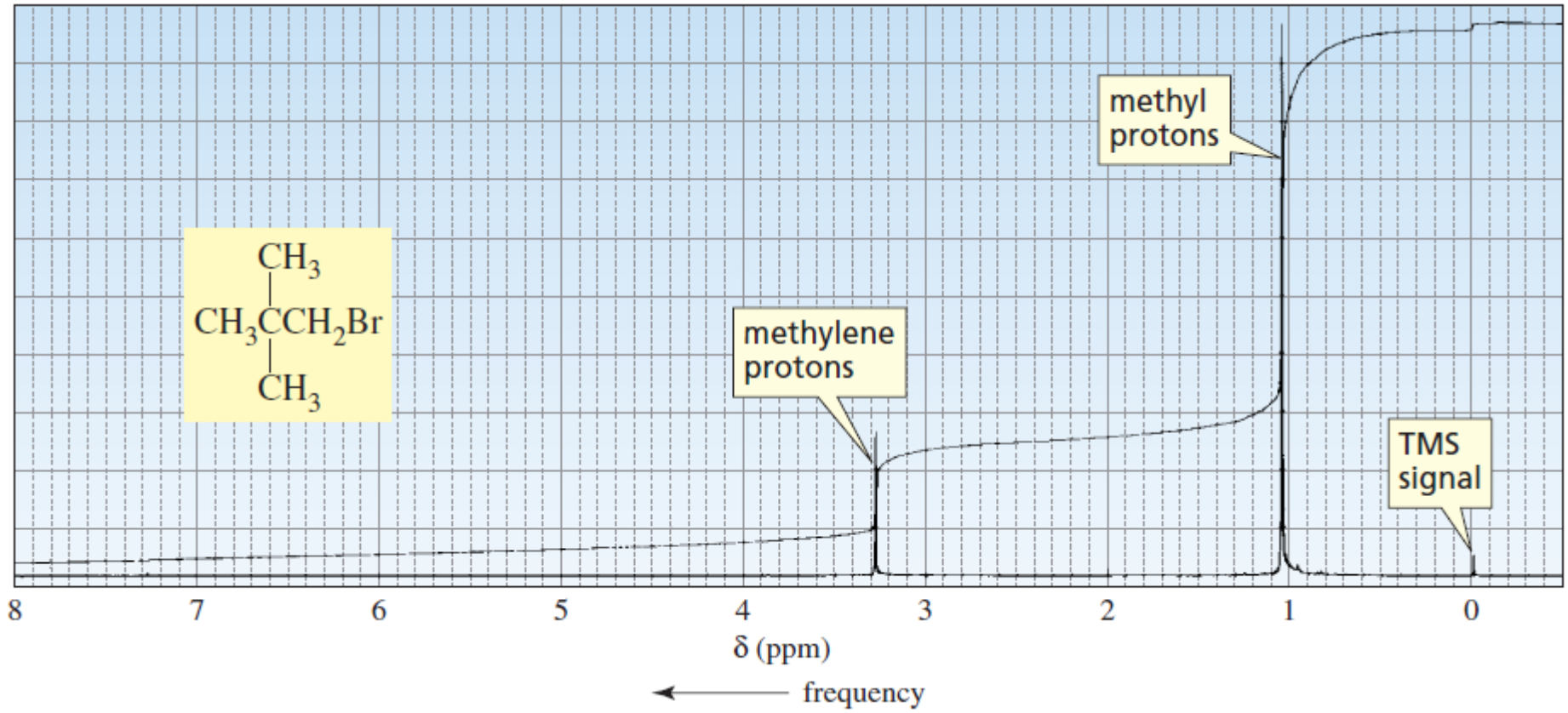
H_c and H_d are not equivalent

Even though they are bonded to the same carbon, the **H_a** and **H_b** protons are not equivalent because they are not in the same environment: **H_a** is trans to Cl and **H_b** is cis to Cl.

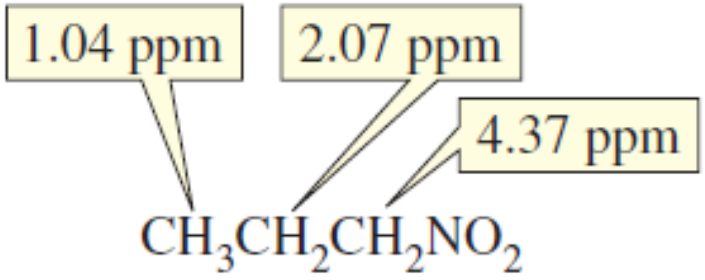
Chemical Shifts

Chemical shifts are measured using TMS as reference compound

Most proton chemical shifts fall in the range from 0 to 10 ppm



The Relative Positions of ^{1}H-NMR Signals



protons in electron-poor environments	protons in electron-dense environments
deshielded protons	shielded protons
downfield	upfield
high frequency	low frequency
large δ values	small δ values

$CH_3CH_2CH_2CH_2CH_2F$ $CH_3CH_2CH_2CH_2CH_2Cl$

$CH_3CH_2CH_2CH_2CH_2Br$ $CH_3CH_2CH_2CH_2CH_2I$

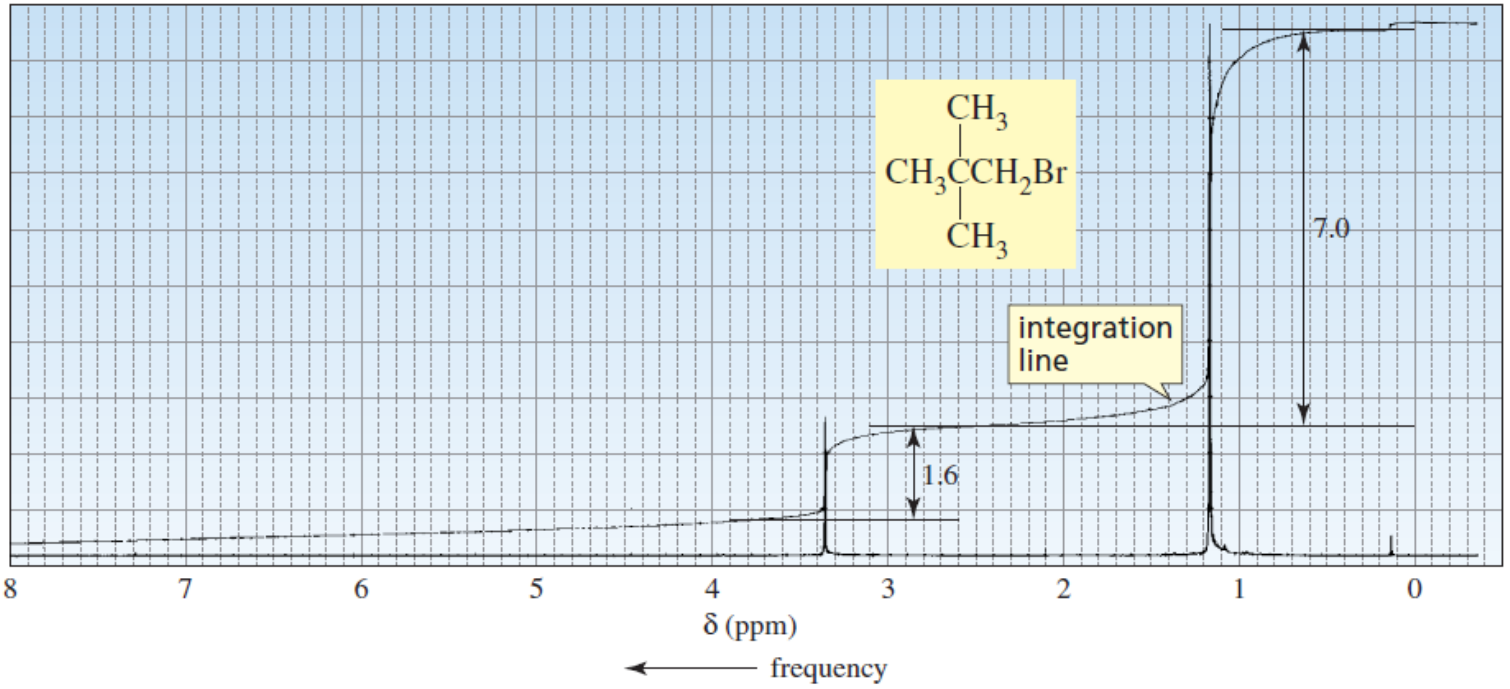
Integration of NMR Signals: Number of Proton

The area under each signal is proportional to the number of protons that gives rise to the signal

Area under a curve can be determined by integration

The integrals can also be displayed by a line of integration superimposed on the original spectrum

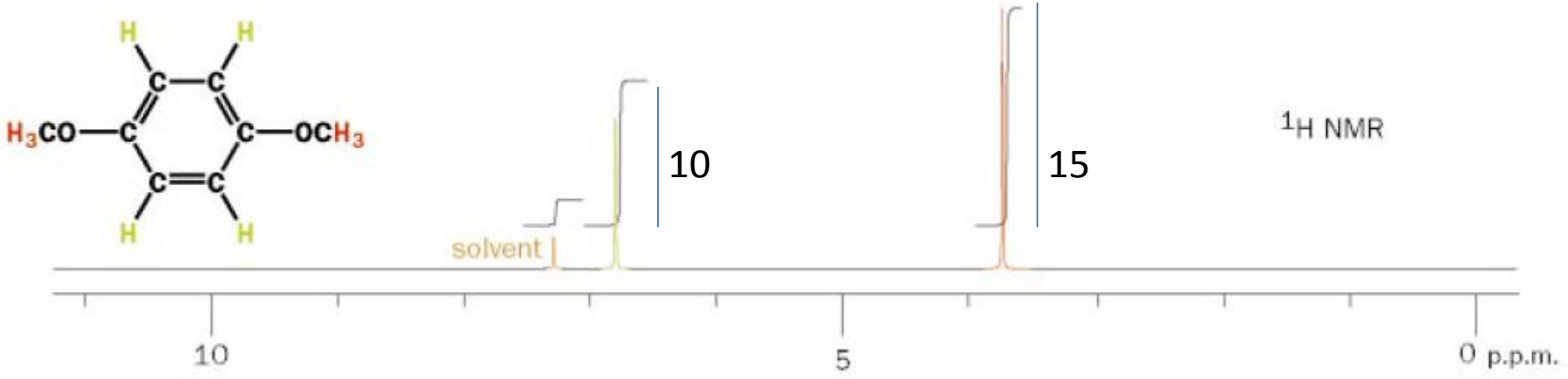
The height of each integration step is proportional to the area under that signal, which, in turn, is proportional to the number of protons giving rise to the signal

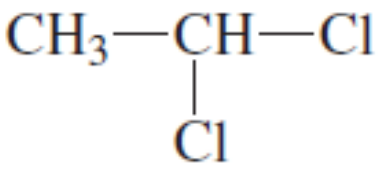


The **integration tells us the *relative number of protons that give rise to each signal,*** not the *absolute number*

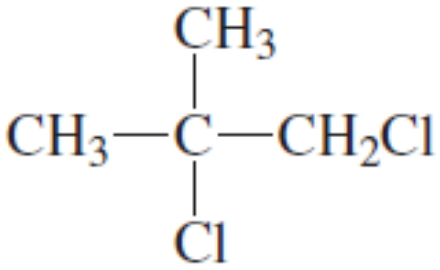
Integration of NMR Signals: Number of Proton

10 : 15 or 2: 3





1,1-dichloroethane
ratio of protons = 1:3



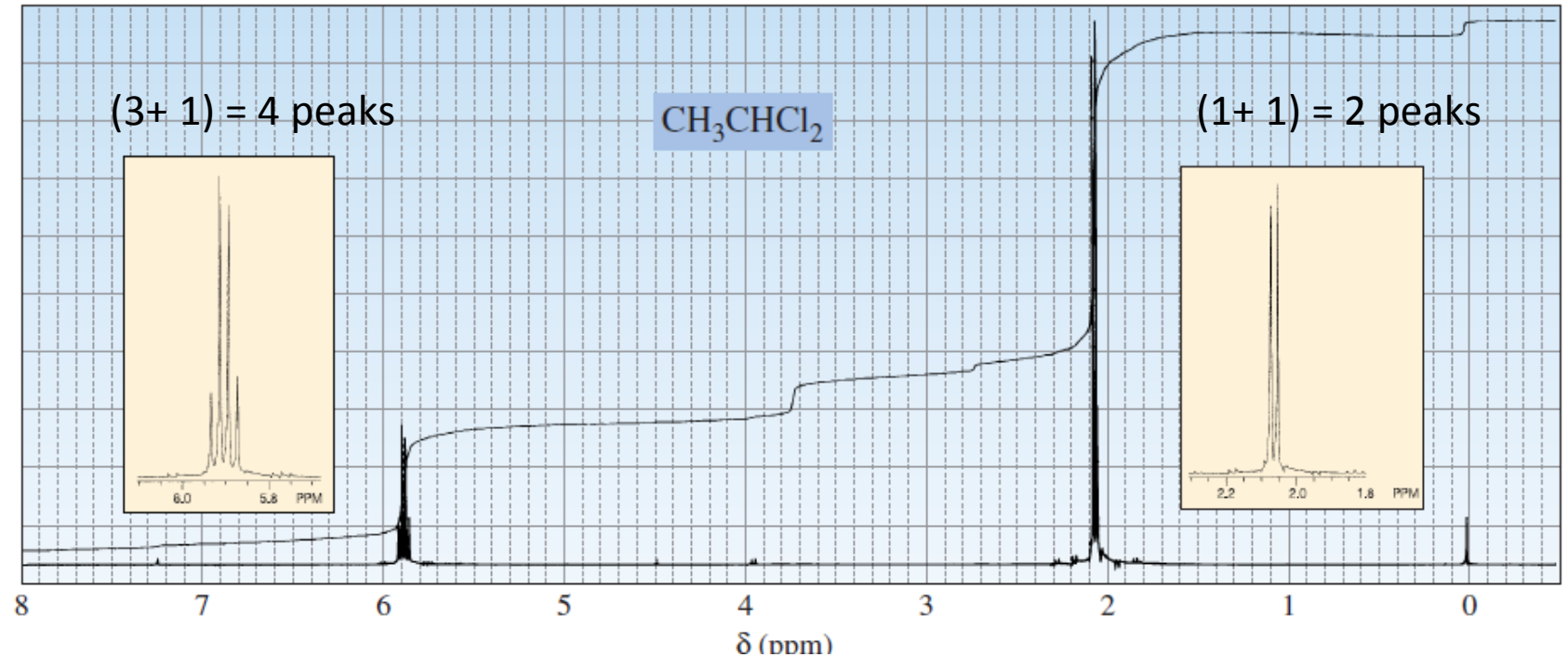
1,2-dichloro-2-methylpropane
ratio of protons 2:6 = 1:3

Coupling in the proton NMR spectrum

Nearby hydrogen nuclei interact and give multiple peaks via spliting the peaks. The interaction between nearby protons known as **coupling.**

Splitting is caused by protons bonded to adjacent (i.e., directly attached) carbons. The splitting of a signal is described by ***N*** + **1**, where *N is the number of equivalent* protons bonded to *adjacent carbons.*

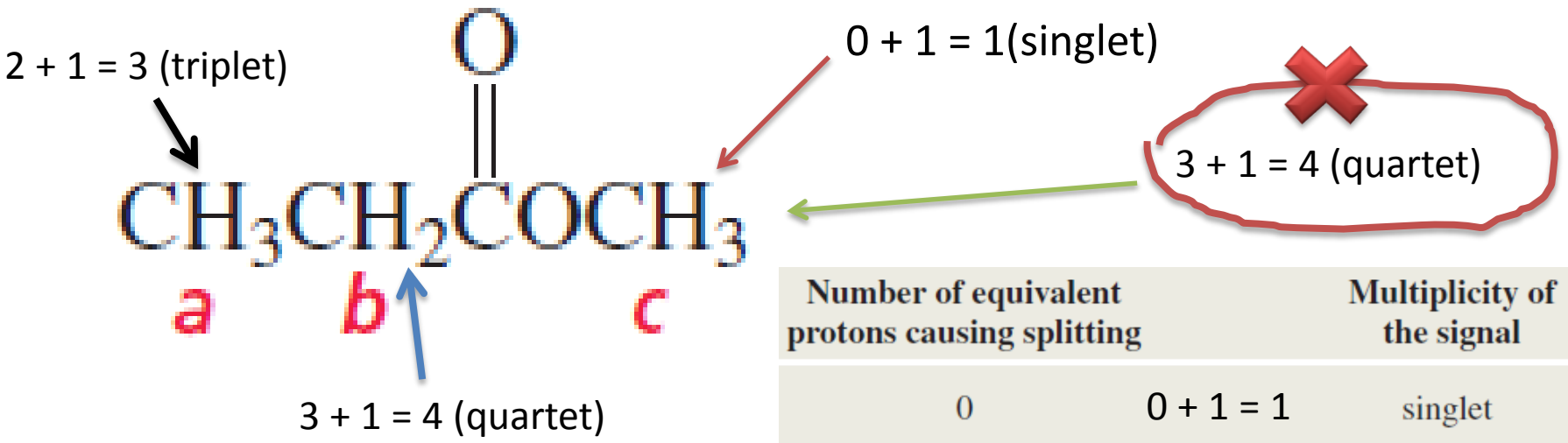
By "equivalent protons," we mean that the protons bonded to an adjacent carbon are equivalent to each other, but not equivalent to the proton giving rise to the signal.



Coupling in the proton NMR spectrum

*it is **not** the number of **protons giving rise to a signal** that determines the multiplicity of the signal*

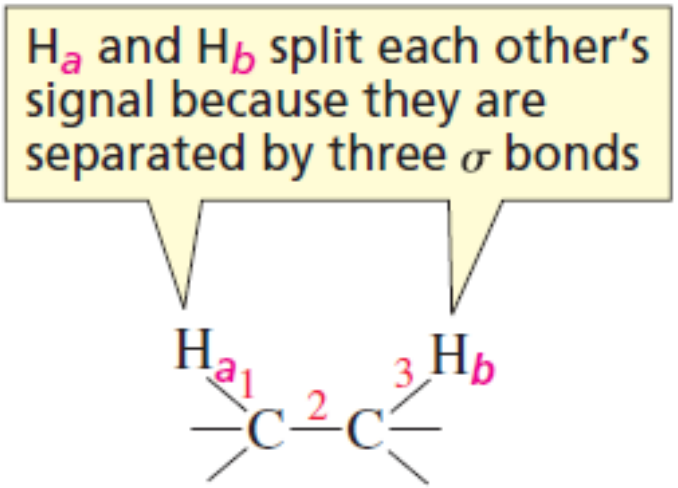
*it **is** the number of protons **bonded to the immediately adjacent carbons** that determines the multiplicity.*

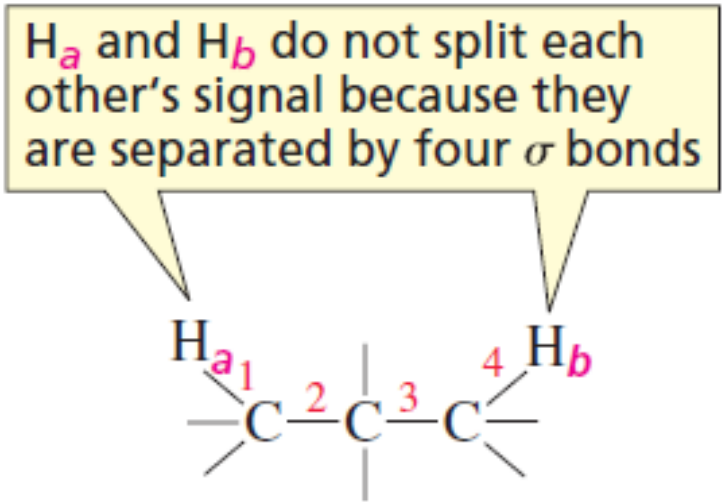


> 7 are considered as multiplet

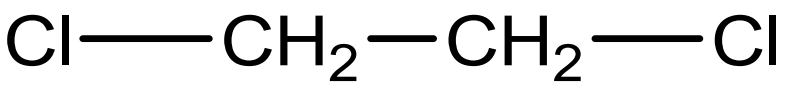
Number of equivalent protons causing splitting		Multiplicity of the signal
0	0 + 1 = 1	singlet
1	1 + 1 = 2	doublet
2	2 + 1 = 3	triplet
3	3 + 1 = 4	quartet
4	4 + 1 = 5	quintet
5	5 + 1 = 6	sextet
6	6 + 1 = 7	septet

Coupling in the proton NMR spectrum





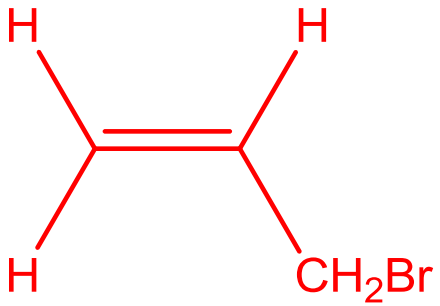
How many signal can be found in 1H-NMR spectrum of the following compound?
What would be the splitting pattern of the signal?



1,2-dichloroethane has an NMR spectrum that shows one singlet

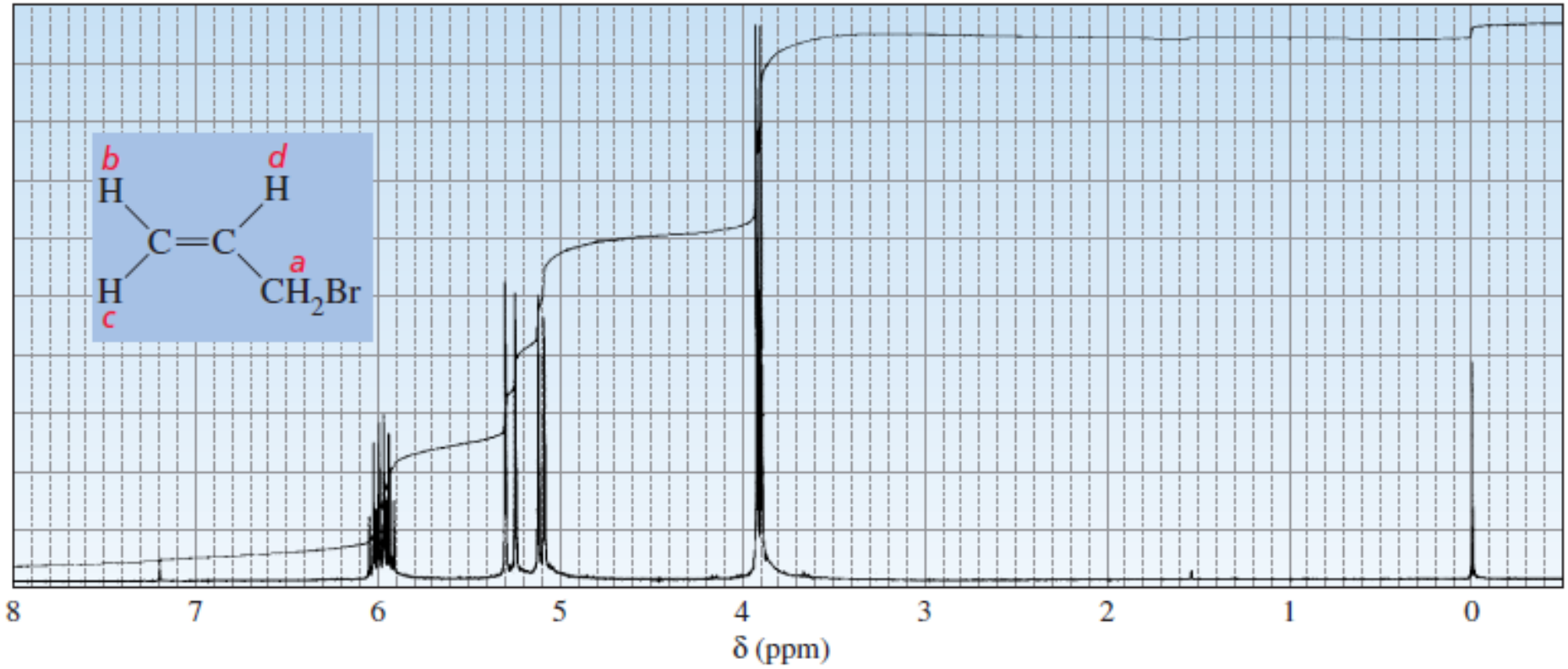
Chemically equivalent protons do not split each other's signal

^{1}H-NMR Spectroscopy

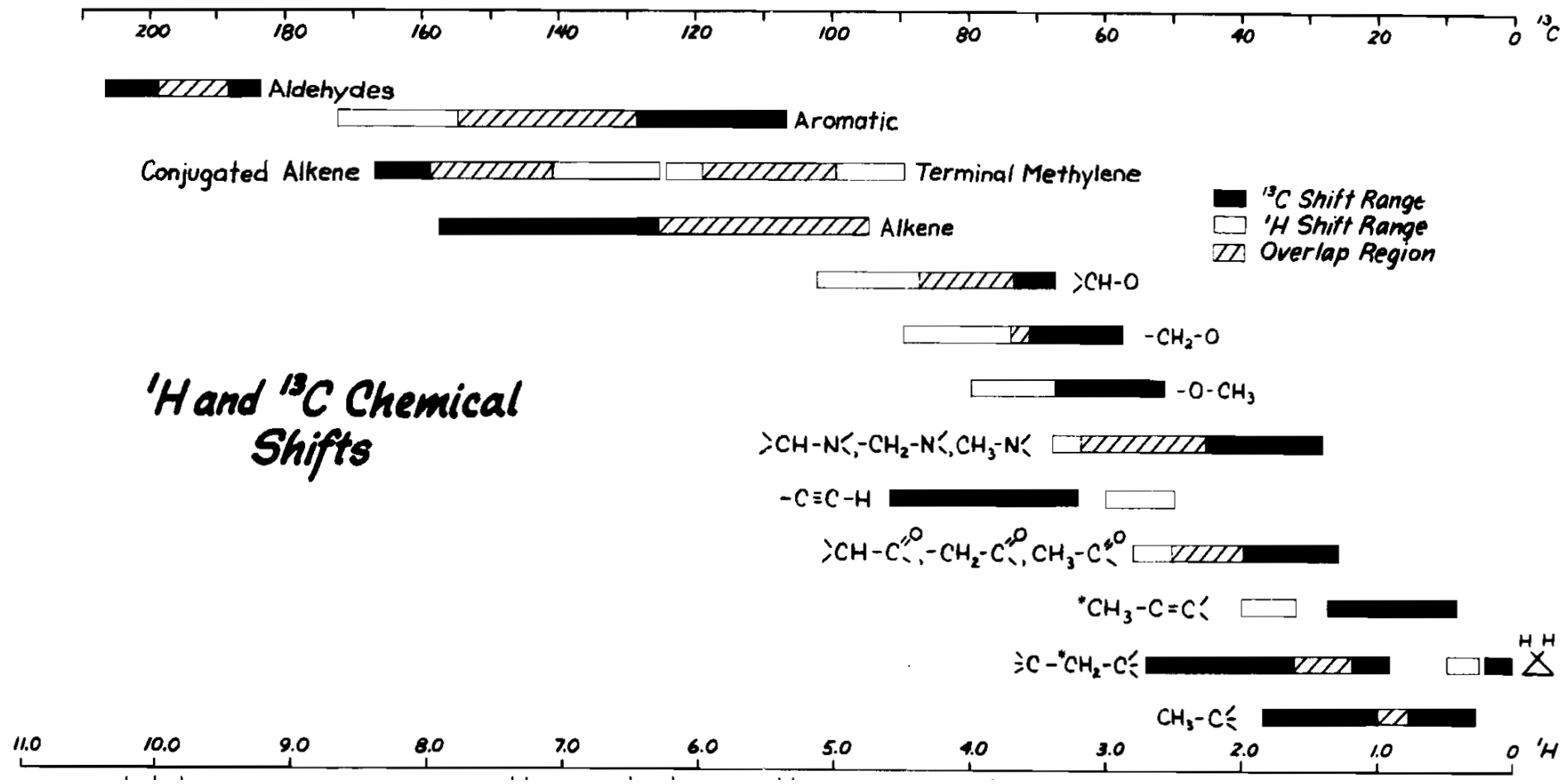


How many signals you expect in 1H-NMR?

What will be the multiplicity of each signal?



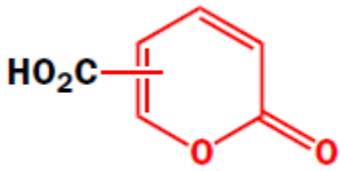
^{1}H-NMR Spectroscopy



^{1}H and ^{13}C Chemical Shifts

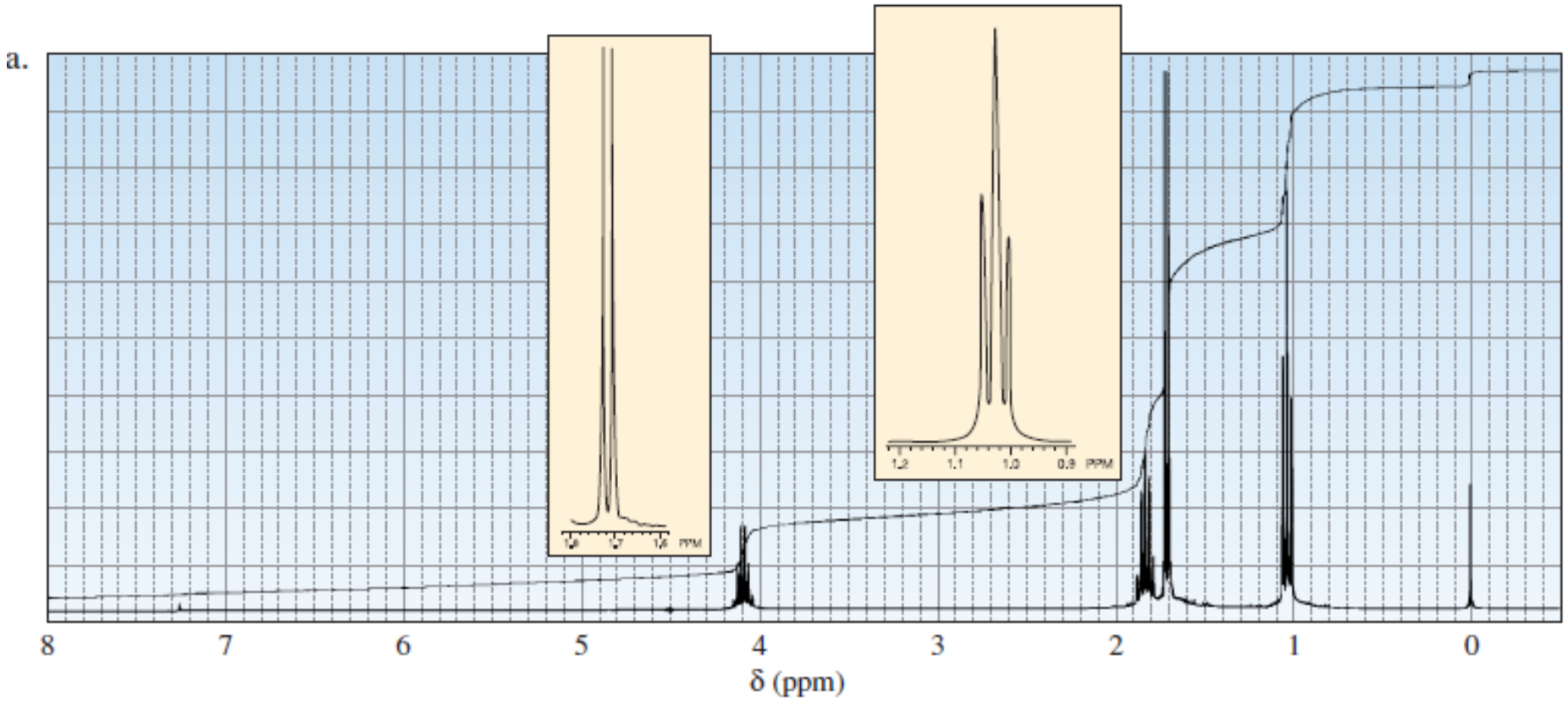
^{1}H-NMR Spectroscopy

One isomer of coumalic acid has the 1H NMR spectrum 6.41 (1H, d), 7.82 (1H, dd*), 8.51 (1H, d).* which isomer is it?



^{1}H-NMR Spectroscopy

The ^{1}H-NMR spectra of one isomers with molecular formula C_4H_9Br is shown here. ^{13}C-NMR of that isomer give four peaks. What is the molecular structure of that isomer ?



Looking forward

End Sem Examination
on
All Topics Discussed