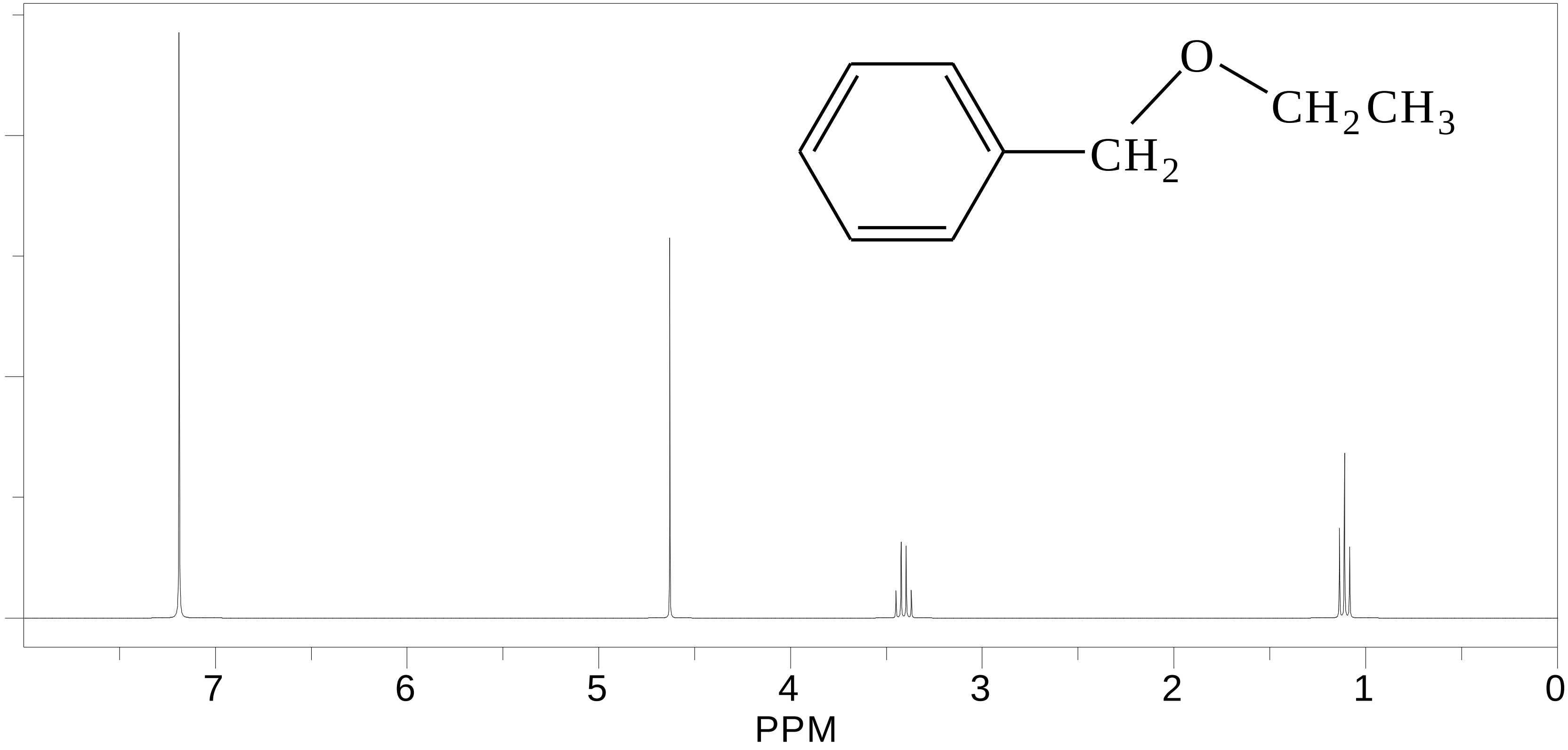
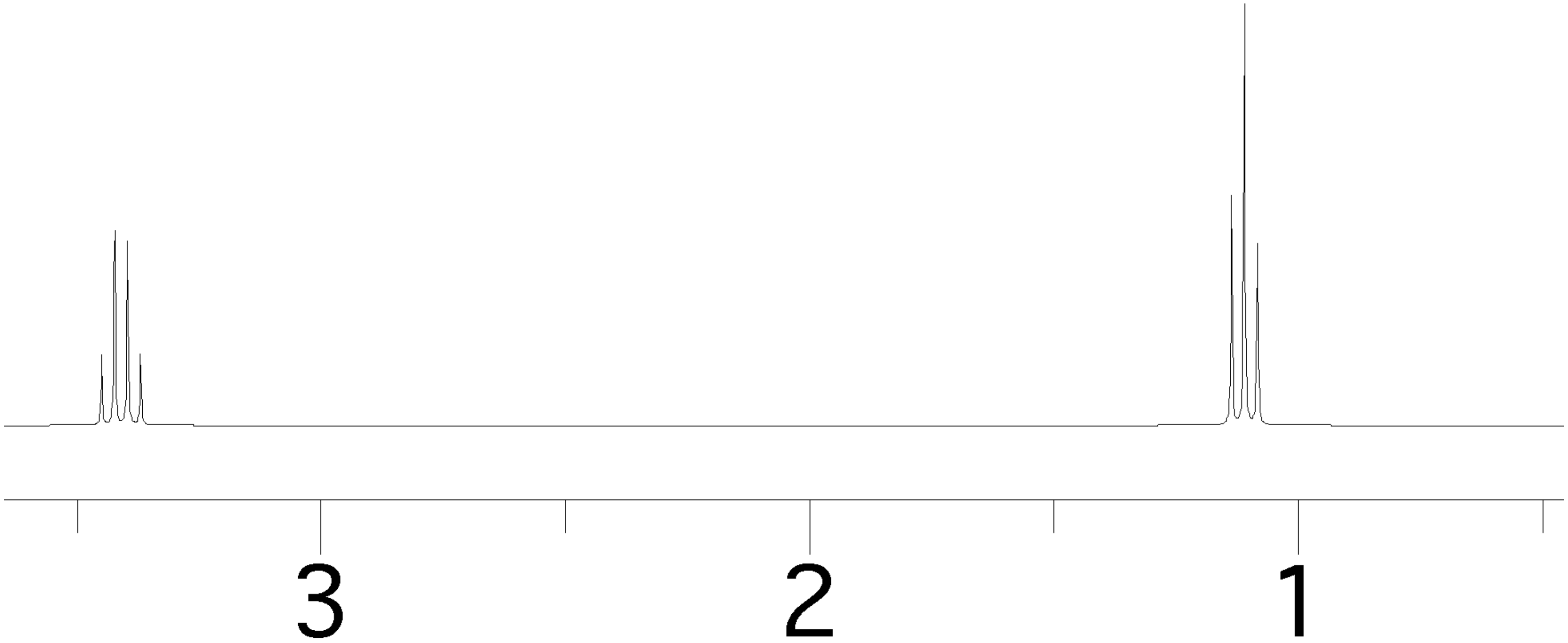
Nuclear Magnetic Resonance (NMR) Spectroscopy



A ^{1}H NMR spectrum. (The plural of spectrum is spectra.)
NMR spectroscopy:

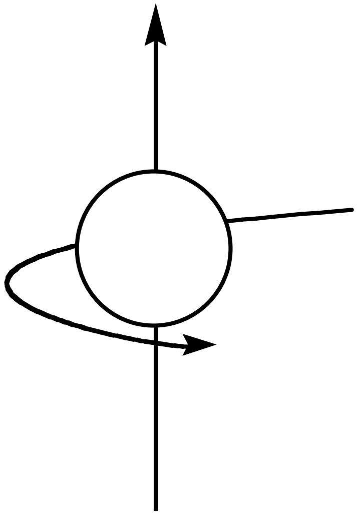
NMR Spectroscopy



- Number of Signals
- Chemical Shift
- Intensity of Signal (Integration)
- Multiplicity

How does NMR spectroscopy work?

- As electrons, protons and neutrons also have spin.
- Thus, most nuclei have a net spin, which is quantized and described by the quantum number, I. (0, ½, 1, $^{3}/_{2}$, 2, $^{5}/_{2}$…)

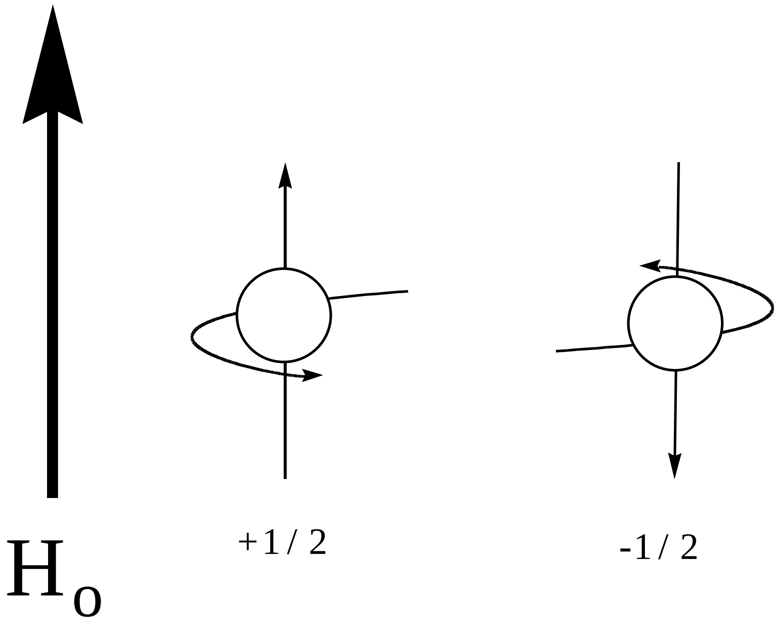


- Spin 0 nuclei: ^{12}C, ^{16}O
- Spin ½: ^{1}H (proton), ^{13}C, ^{15}N, ^{19}F, ^{29}Si, ^{31}P, ^{77}Se, ^{89}Y, ^{103}Rh, ^{125}Te, ^{129}Xe, ^{195}Pt
- Spin 1 nuclei: ^{2}H, ^{6}Li, ^{14}N
- Spin $^{3}/_{2}$ nuclei: ^{7}Li, ^{11}B
- Spin $^{5}/_{2}$ nuclei: ^{17}O
- Spin 3 nuclei: ^{10}B

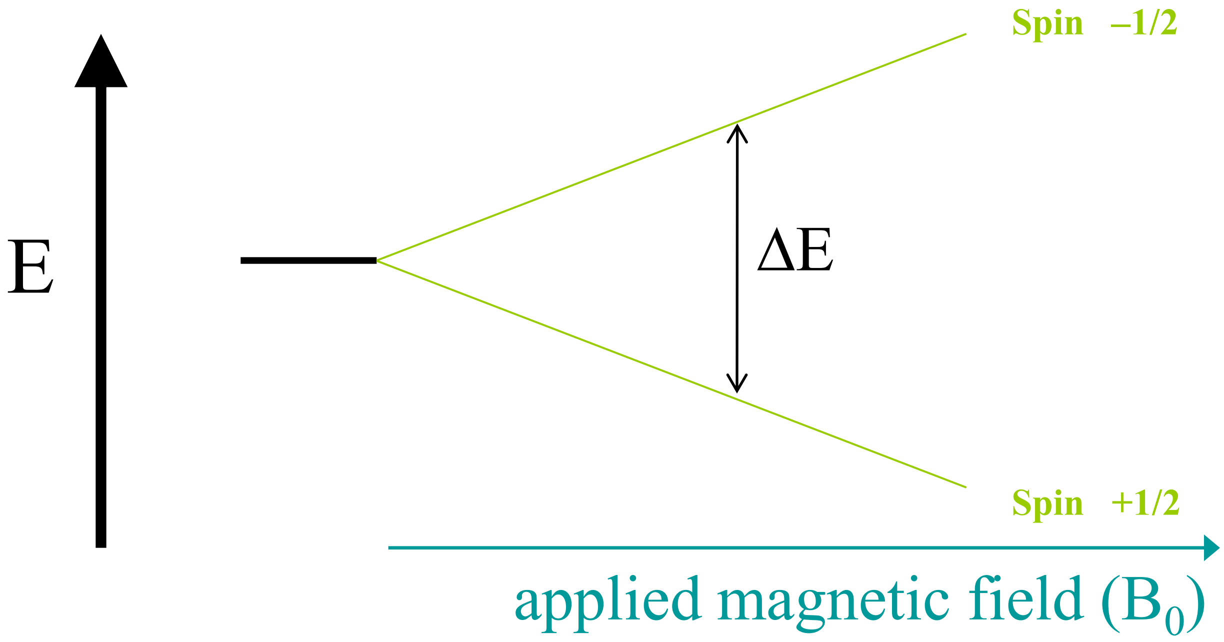
- In a given sample of a compound in solution, spins are random.
    - the sample has no net spin due to averaging

- In the presence of an externally applied magnetic field (H_o), a nucleus will adopt 2I + 1 orientations with differing energies.

- For the proton, there are two “spin states”.
    - each spin state has a slightly different energy level



Zeeman splitting:



Important:

- The relative number of nuclei in the different spin states (^{1}H, 300 MHz) is:

$$\frac{N_{upper}}{N_{lower}} = e^{\frac{-\Delta E}{kT}} = \frac{1{,}000{,}000}{1{,}000{,}048}$$

$$\Delta E = h\nu = \frac{h\gamma}{2\pi} H_o$$

$$\nu = \frac{\gamma}{2\pi} H_o$$

- The magnetogyric ratio, γ, is a physical constant for each nucleus.

Nucleus	radians/Tesla*
^{1}H	267.53
^{2}H	41.1
^{13}C	67.28
^{19}F	251.7
^{31}P	108.3

*1 Tesla = 10,000 Gauss.

- Thus, ΔE depends on…

- Resonance occurs when…

NMR Spectroscopy

For the proton nucleus:

	H_o	ν
•	1.410 Tesla	60 MHz
•	5.874 Tesla	250 MHz
•	11.750 Tesla	500 MHz

But…

…the actual resonance frequency for a given nucleus depends on its…

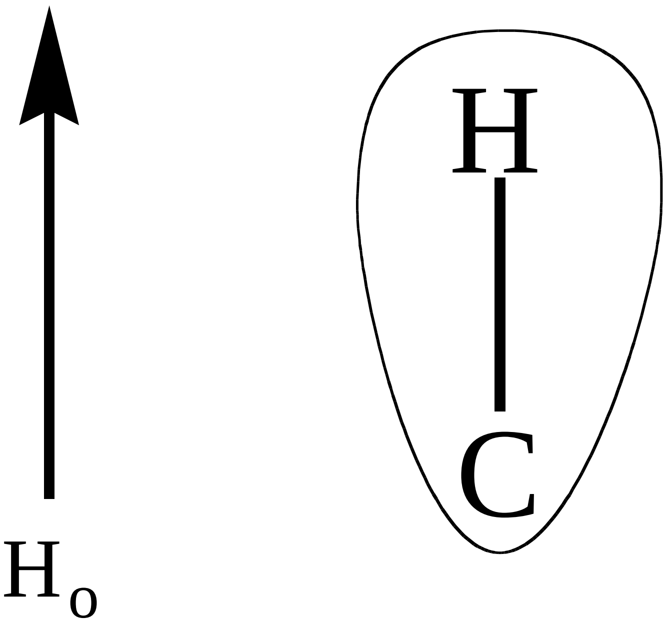
i.e. magnetic interactions within the molecule.

NMR Spectroscopy

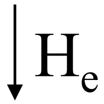
These local magnetic effects are due to:

- σ electrons
- π electrons
- other nuclei – especially protons

σ electrons

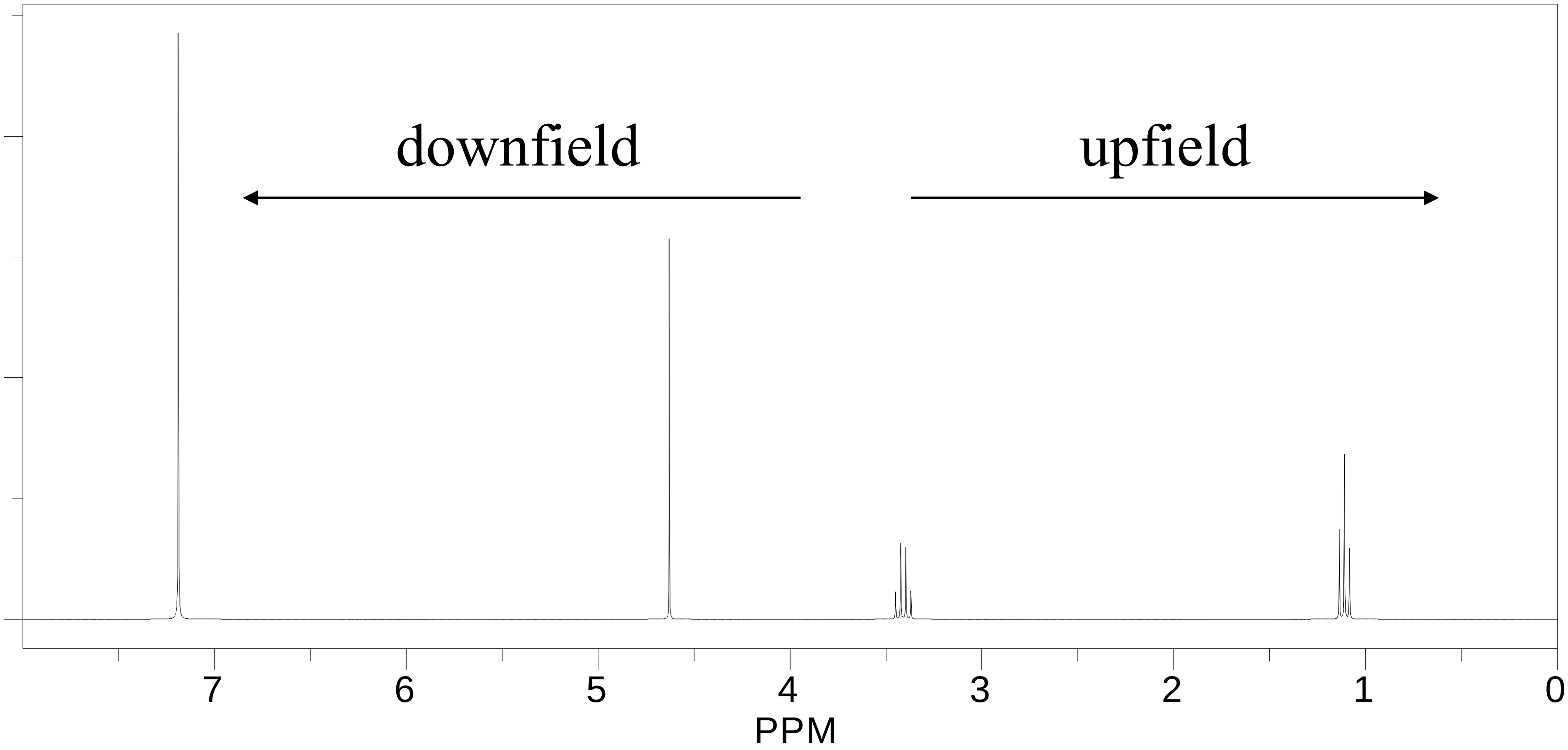


- In the locale of the proton, the field lines are opposed to the applied magnetic field. This has the effect of "shielding" the proton from the full H_o.

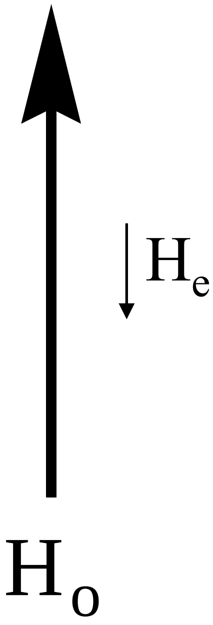


NMR Spectroscopy

- Chemical shielding has the effect of moving signals to the right on an NMR spectrum. We refer to this as…

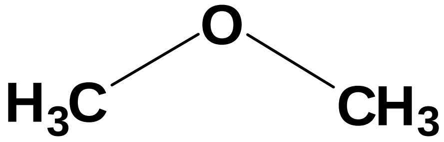


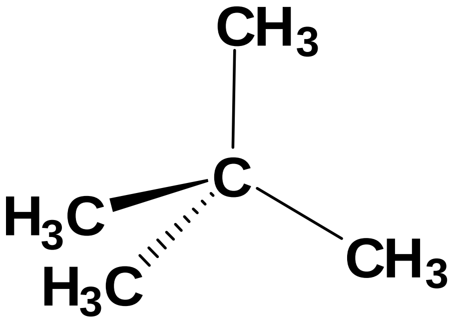
NMR Spectroscopy

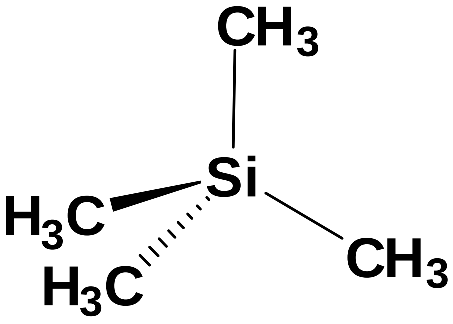


- The magnitude of H_e is proportional to the electron density in the σ bond.

Consider…







Tetramethylsilane
aka TMS

NMR Spectroscopy

- Because almost all proton resonance frequencies (in organic compounds!) are found downfield of the TMS signal, TMS is used as an internal reference. All peak positions are measured as frequencies in Hz downfield of TMS, with TMS at zero.

- There is a problem however..

…ν is proportional to H_o

For example:

H_o = 60 MHz, ν = 210 Hz downfield of TMS

H_o = 100 MHz, ν = 350 Hz downfield of TMS

NMR Spectroscopy

- Solution to this problem…

We define the δ scale:

$$\delta = \frac{\nu_{\text{signal downfield of TMS}}}{\text{spectrometer frequency in MHz}} = ppm$$

NMR Spectroscopy

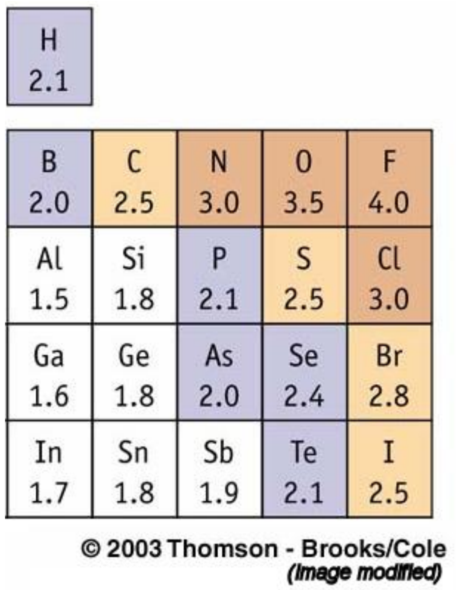
- In an alkane, chemical shifts depend on whether the ^1H is attached to a primary, secondary or tertiary carbon:

CH_4	0.23 ppm
CH_3CH_3	0.86 ppm
$CH_3CH_2CH_3$	0.91 & 1.37 ppm
2-methylpropane	0.96 & 2.01 ppm

NMR Spectroscopy

- Chemical shift correlates well with electronegativity…

$$H_3C-X$$



H 2.1				
B 2.0	C 2.5	N 3.0	O 3.5	F 4.0
Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0
Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8
In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5

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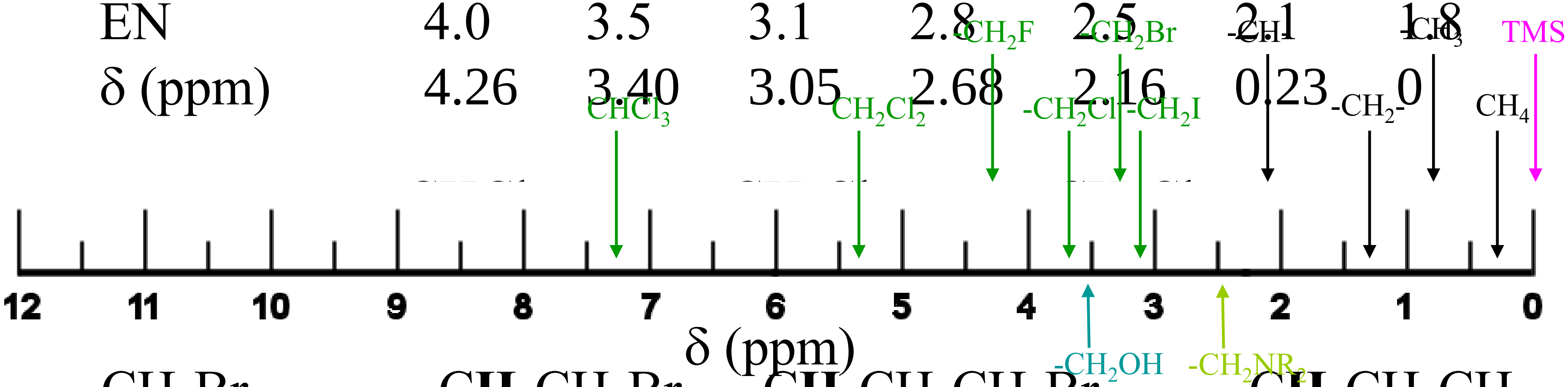
(image modified)

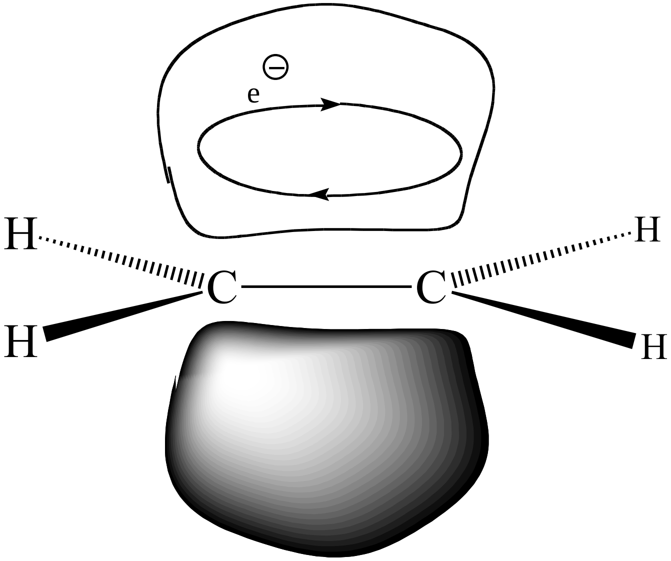
	F	O	Cl	Br	I	H	TMS
EN	4.0	3.5	3.1	2.8	2.5	2.1	1.8
δ (ppm)	4.26	3.40	3.05	2.68	2.16	0.23	0

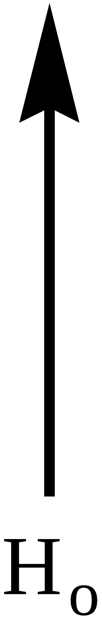


–CH_2Br	–C$\underline{\mathbf{H_2}}$$CH_2Br$	–C$\underline{\mathbf{H_2}}$$CH_2CH_2Br$	–C$\underline{\mathbf{H_2}}$$CH_2CH_3$
3.30	1.69	1.25	1.20

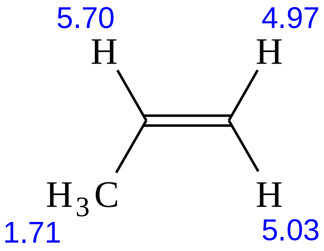
π–Electron Effects – Diamagnetic Anisotropy

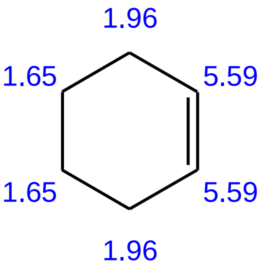
Alkenes…

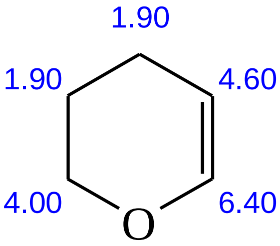


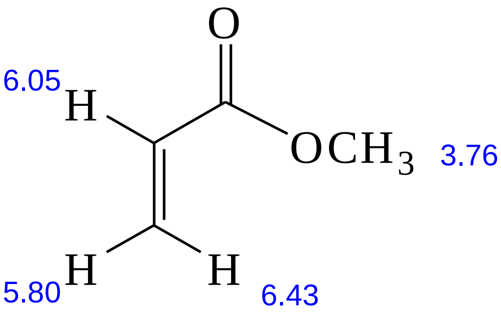


Vinyl protons are downfield, 4.5 - 6 ppm.



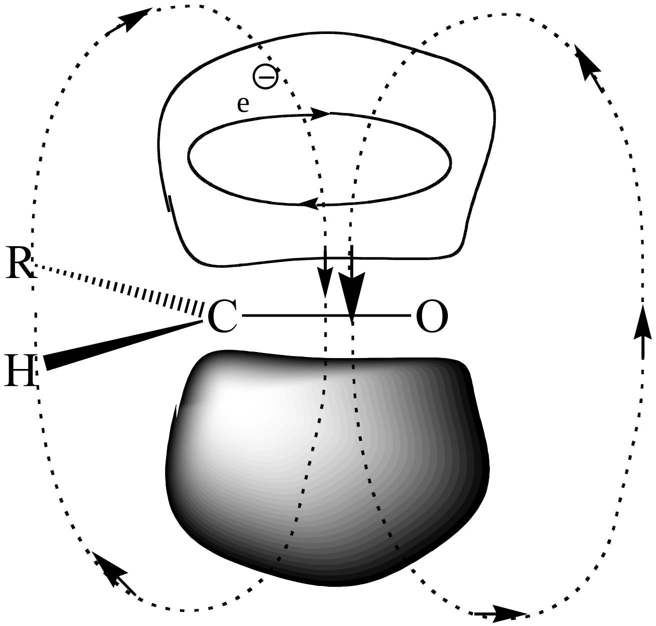


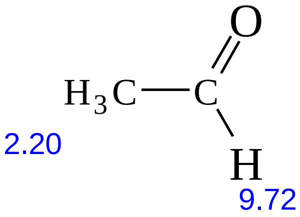


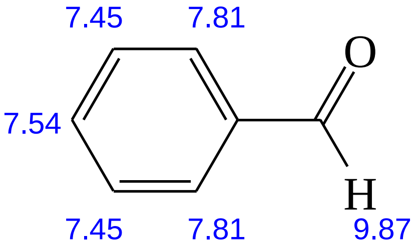


π–Electron Effects – Diamagnetic Anisotropy

Aldehydes

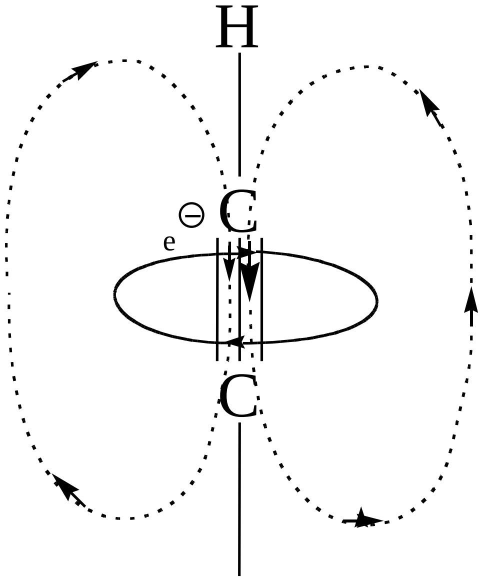




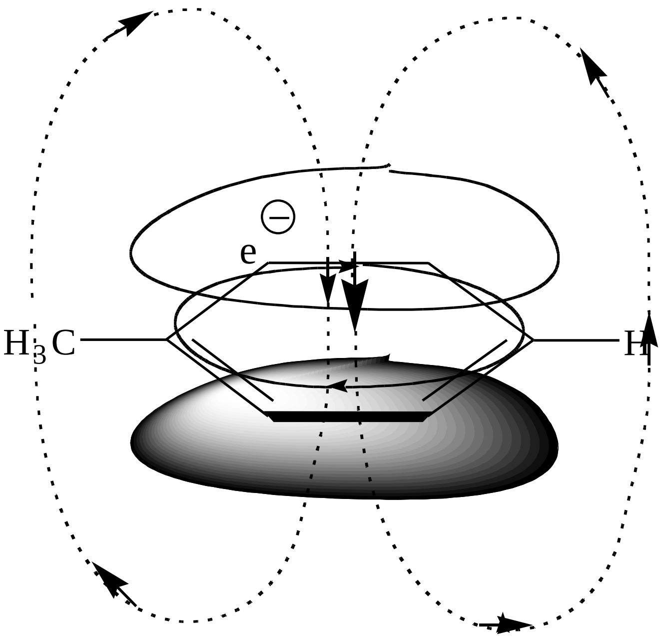


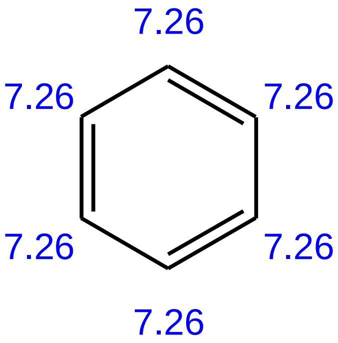
Alkynes

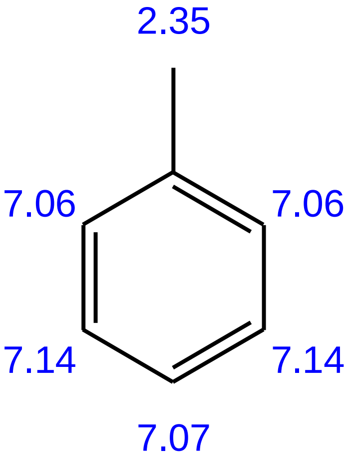
1.80 $H_3C—C \equiv C—H$ 1.82



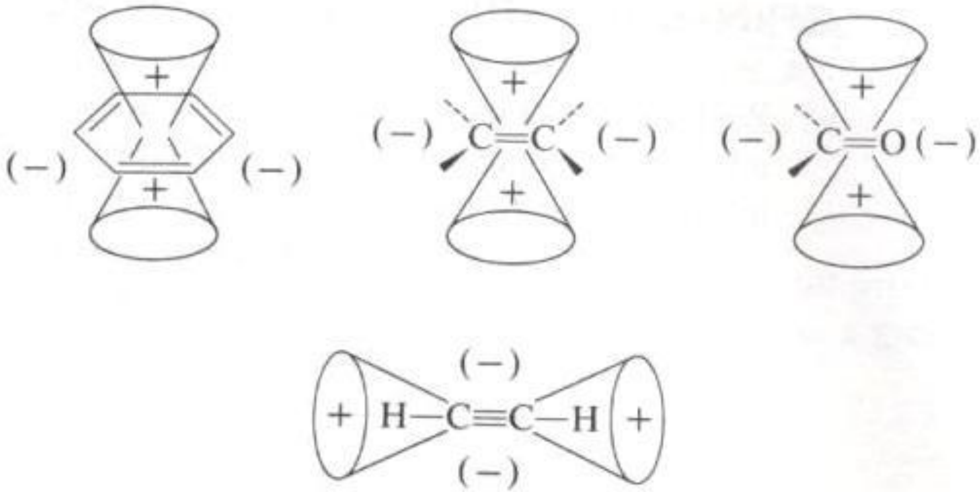
π–Electron Effects – Diamagnetic Anisotropy





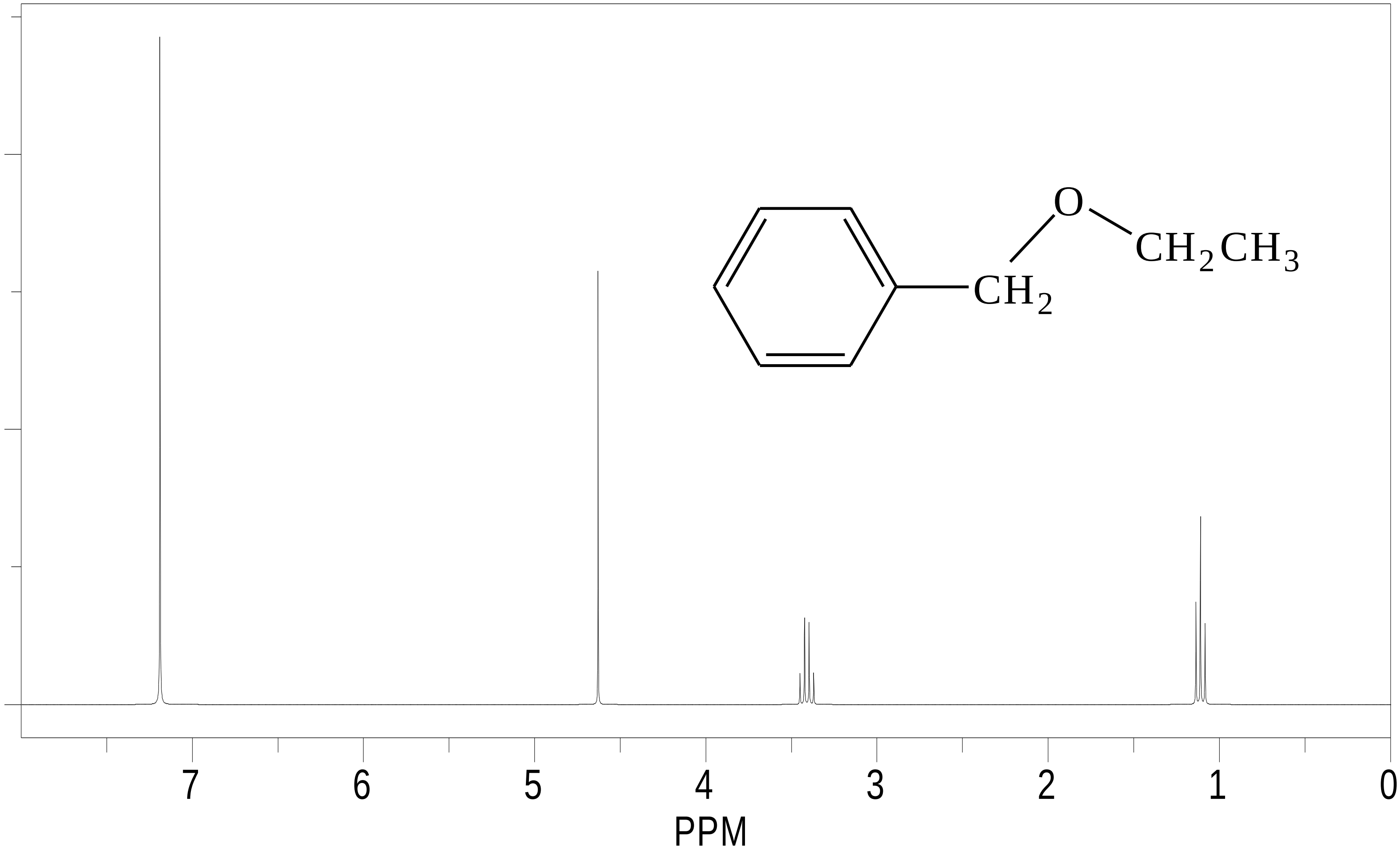


Brief Summary of π Bonds & Anisotropic Effects

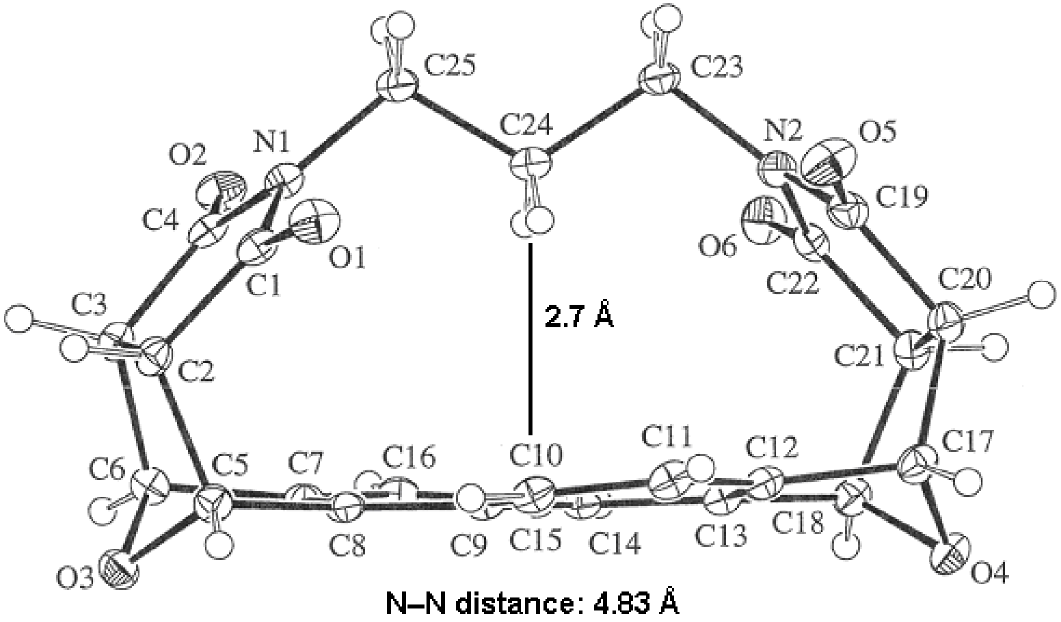


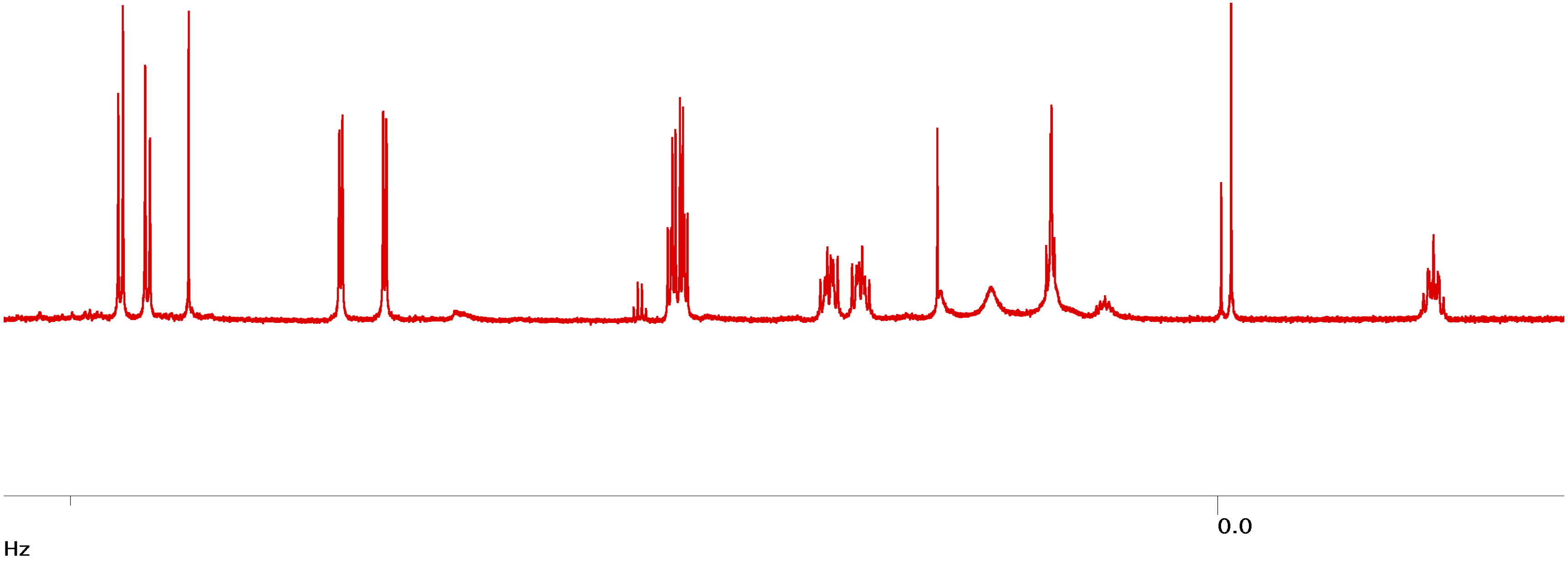
▶ **FIGURE 3.23** Anisotropy caused by the presence of π electrons in some common multiple-bond systems.

NMR Spectroscopy

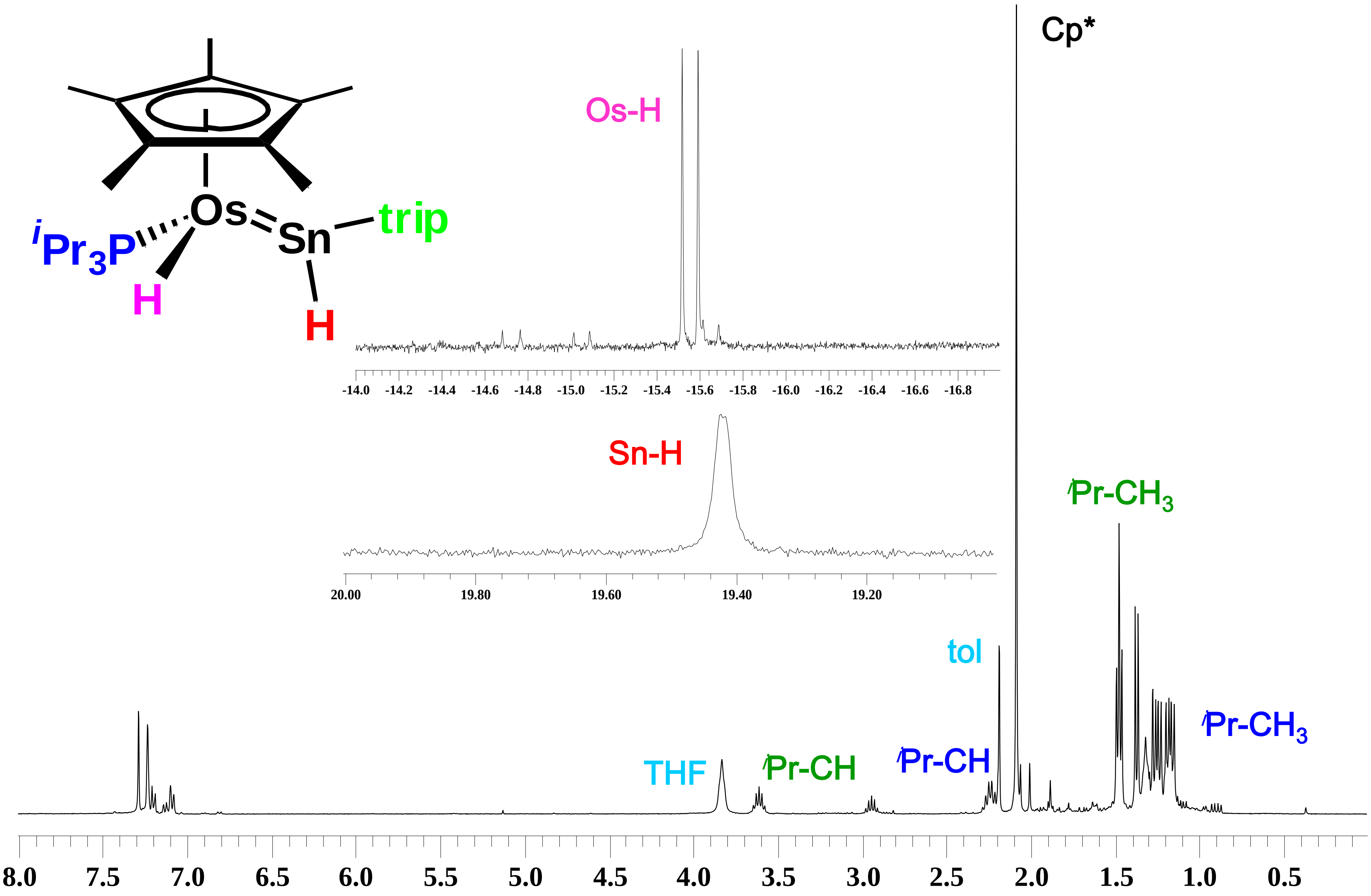


X-ray Structure of the 3C Naphthodifuran Cyclophane (Prof. Dibble)

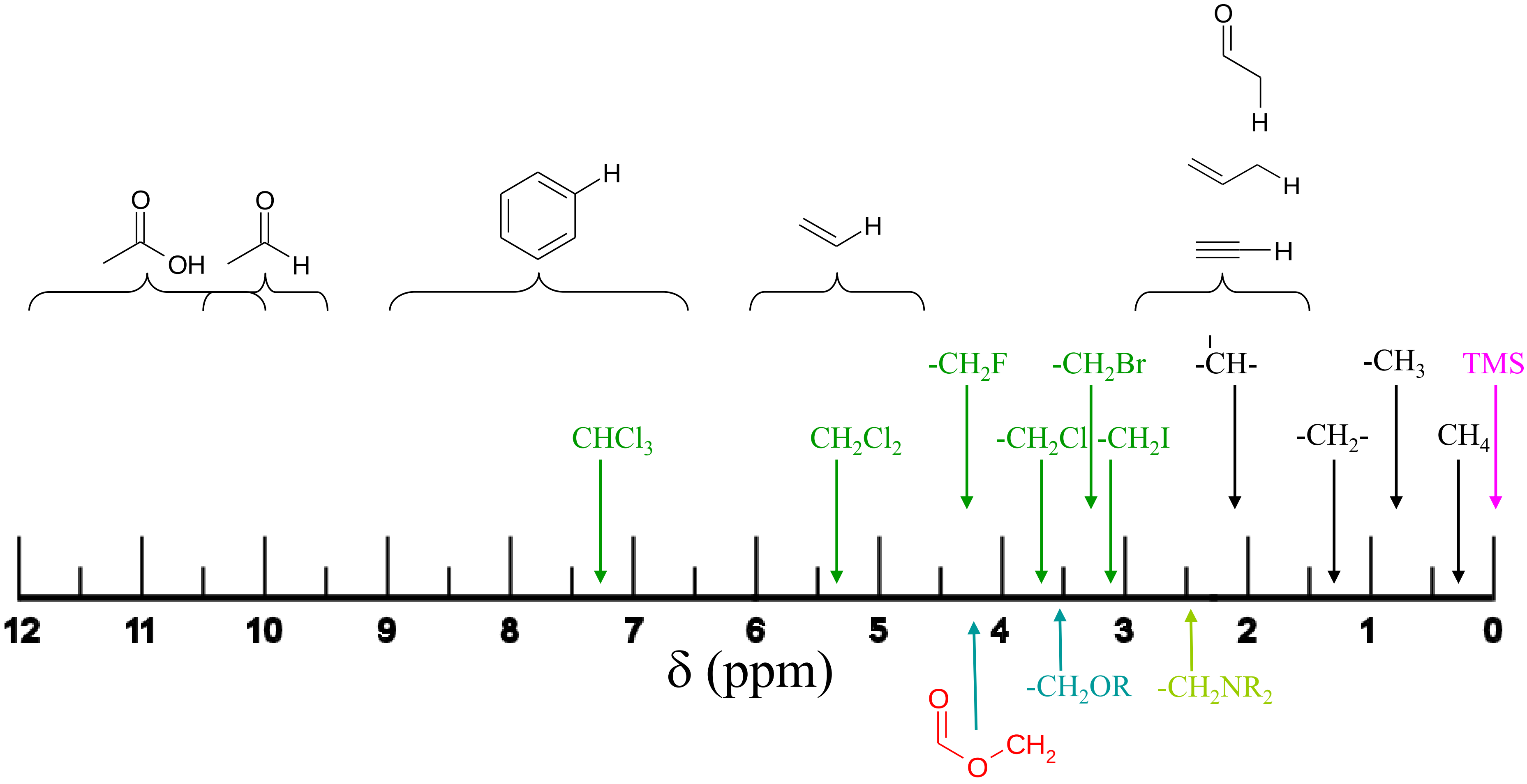




Osmium Stannylene Complex



Chemical Shifts Summary

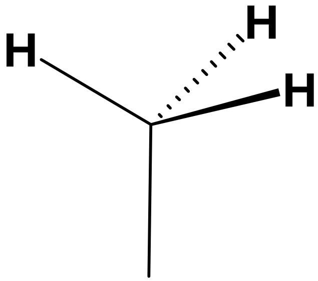


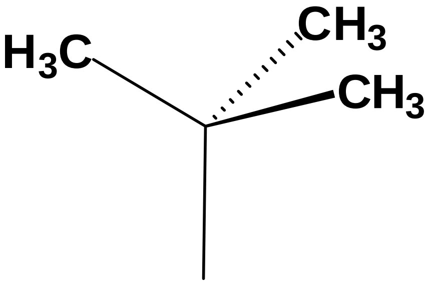
- NH and OH can appear anywhere between 0 and 14 ppm!
- Only carboxylic acids are somewhat consistent in their chemical shift.
- NH and OH peaks are often very broading and lack expected multiplicity

Chemical shift equivalence (*i.e.* Number of Signals)

… of atoms or groups.

- Groups or nuclei are shift equivalent if they can be exchanged by a bond rotation without changing the structure of the molecule.



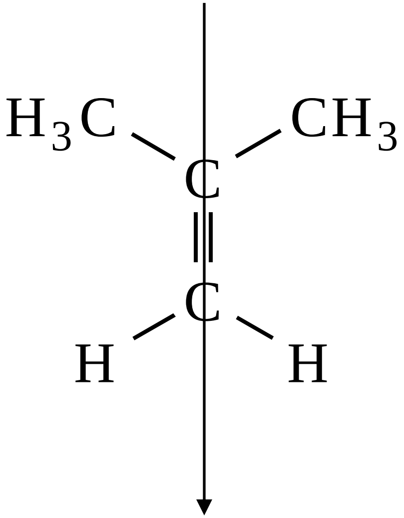


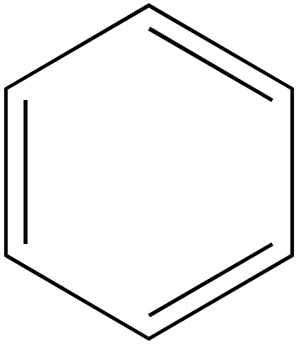
- These atoms/groups are said to be "**<u>homotopic</u>**".
Homotopic atoms/groups are always shift equivalent.

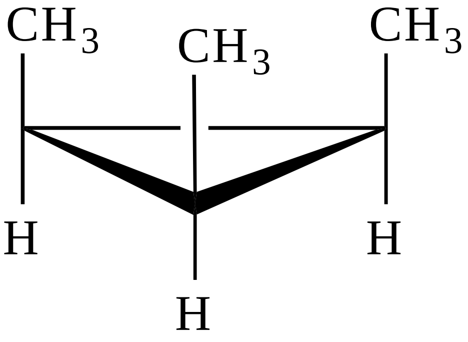
Chemical shift equivalence (*i.e.* Number of Signals)

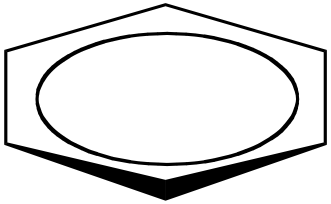
- Shift equivalence can also be determined by symmetry properties of the molecule.

- A proper axis of rotation…



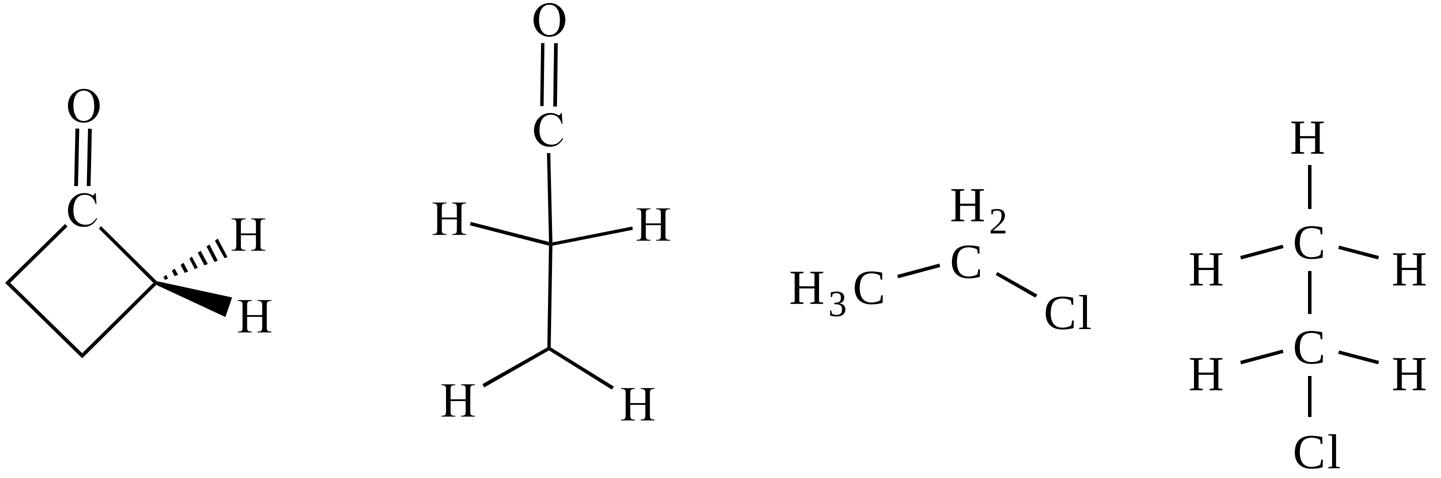






Chemical shift equivalence (*i.e.* Number of Signals)

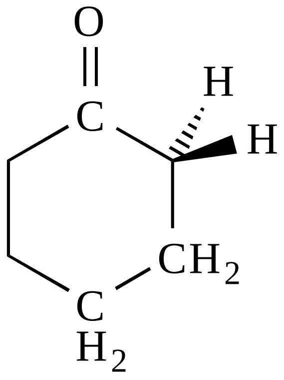
- Atoms/groups that can be reflected in an internal mirror plane of symmetry, but not exchanged by bond rotation or a proper axis of symmetry are “enantiotopic”.

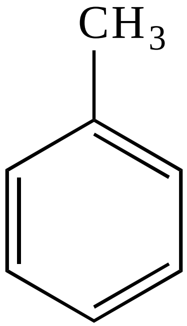


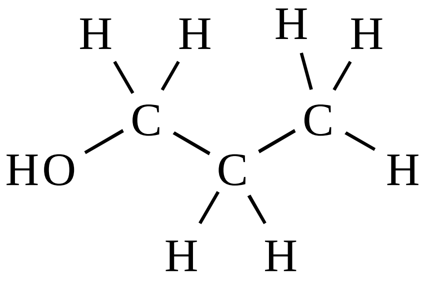
- For our current purposes, enantiotopic protons are always shift equivalent.

Chemical shift equivalence (*i.e.* Number of Signals)

- It is easy to recognize atoms/groups that are constitutionally different.

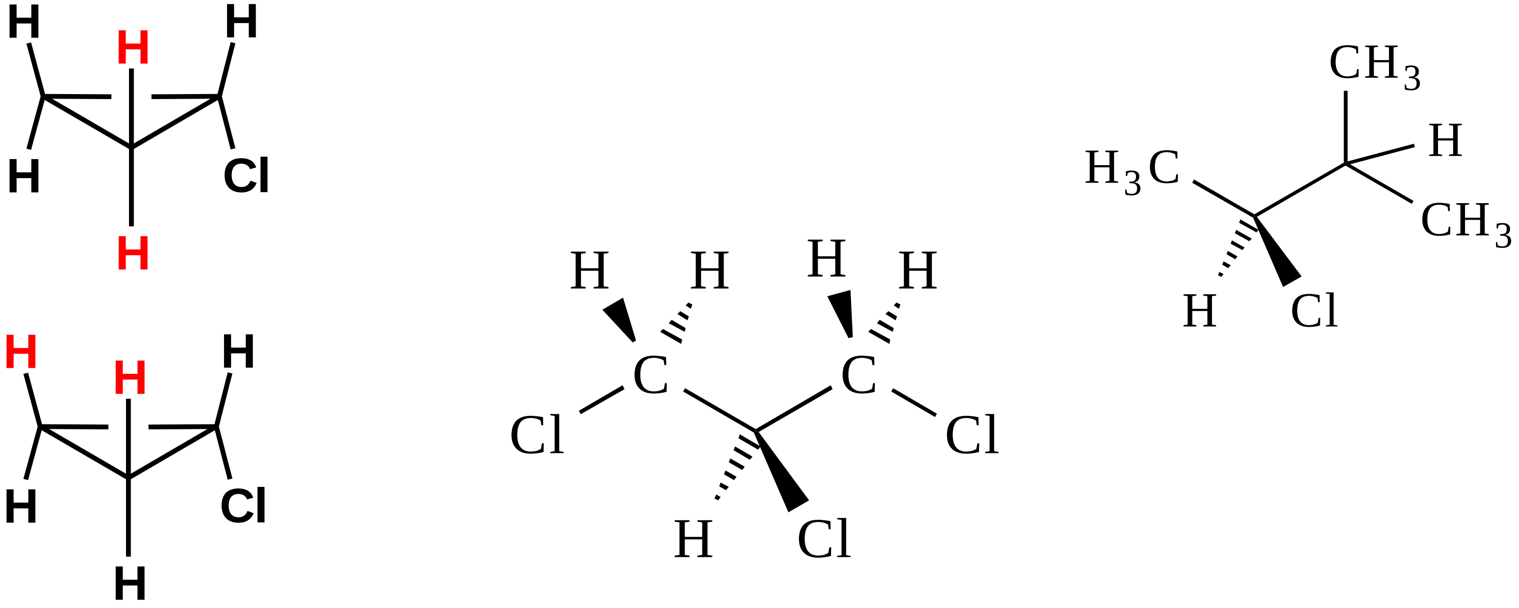






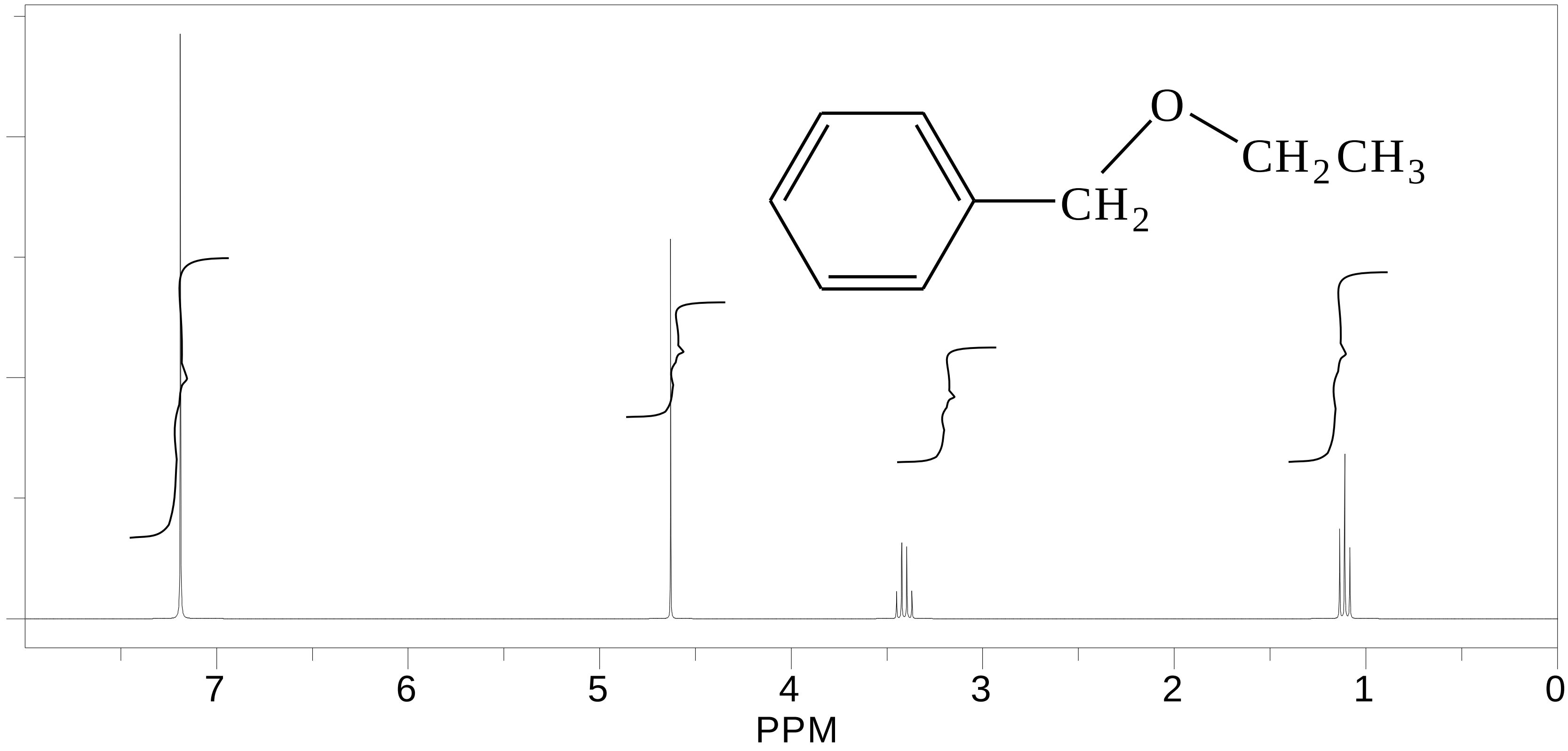
Chemical shift equivalence (*i.e.* Number of Signals)

- Protons that are not constitutionally different, that cannot be exchanged by bond rotation or by molecular symmetry are "**diastereotopic**".



- Diastereotopic atoms/groups are **NOT** shift equivalent, except by coincidence (*i.e.* they happen to have the same chemical shift by accident).

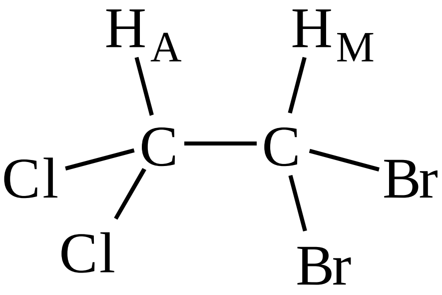
Signal Intensity - Integrations



Raw integrals: 8.5:3.5:3.4:5.0

Other nuclei - spin-spin coupling (Multiplicity)

- Consider the vicinal protons in the molecule:



- In the absence of any influence by H_M, H_A will resonate at ν_A.

- But H_M generates its own magnetic field which will affect ν_A. Is this field aligned with H_o or against H_o (*i.e.* will it shield or deshield H_A)?

Other nuclei - spin-spin coupling (Multiplicity)

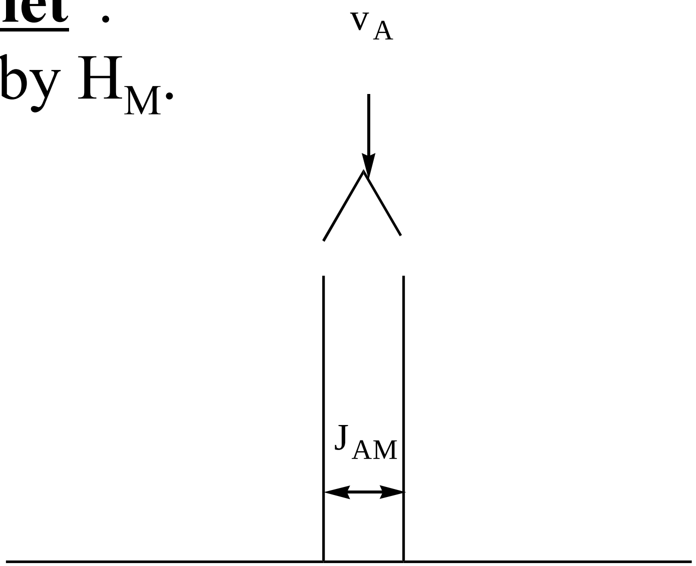
- Remember that the population of the two spin states are nearly equal. In the total of all molecules, half of the H_M protons will be aligned with H_o and half against.

- So in half the molecules, H_M shields H_A and in half H_M deshields H_A. We therefore see two peaks for H_A, of equal intensity; one upfield of ν_A and one downfield of ν_A.

- We call this type of signal a … "**doublet**".
We say that H_A is "split" into a doublet by H_M.

- This effect is referred to as … "**spin-spin**" or J coupling.

- The distance between the two peaks in Hz is J, the **coupling constant**.



Important aspects of coupling:

- Coupling always goes both ways. If H_A is split by H_M, then H_M must also be split by H_A and *J* must be equal in both cases.
- *J*-coupling is a through-bond and not a through-space effect (dipolar coupling).
- Coupling between shift-equivalent nuclei is not observed.

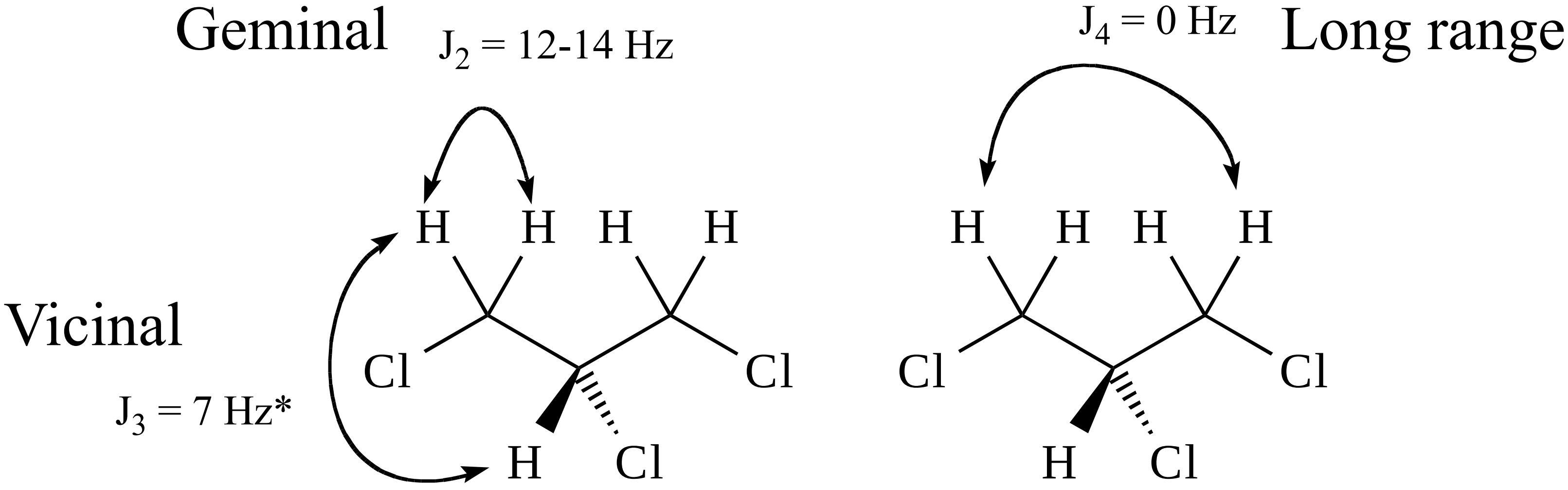
A few words about *J*.

- The magnitude of *J* can be extremely useful in determining structure. It depends on:

  - number of bonds between nuclei
  - type of bonds between nuclei
  - type of nuclei
  - conformation /stereochemistry

A few words about *J*.

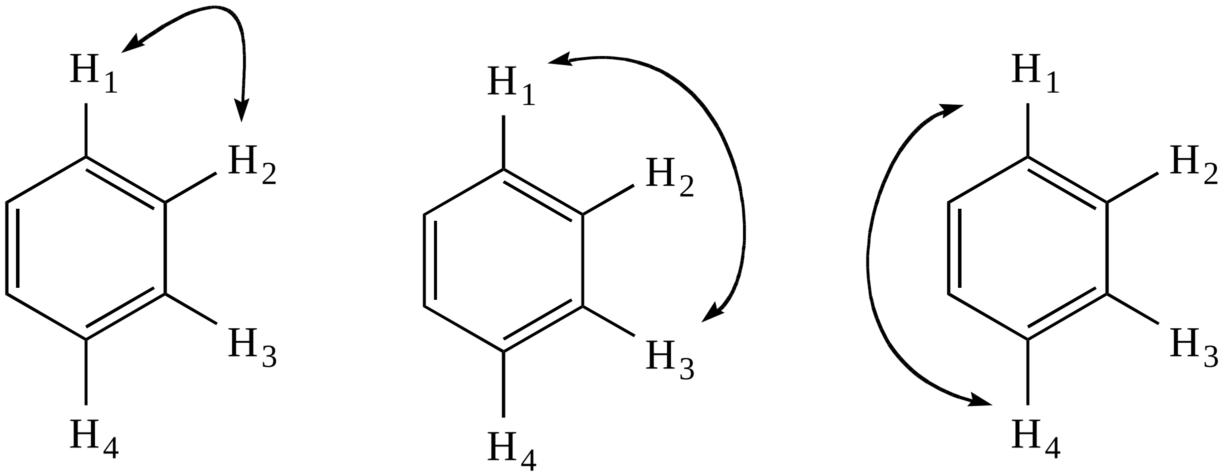
- Because coupling is a through bond effect, the magnitude of *J* depends on the number of bonds between coupling nuclei.
- One bond couplings are typically larger than two bond couplings, two larger than three, etc.
- In ^{1}H-^{1}H couplings, four bond couplings are **usually** not observed.

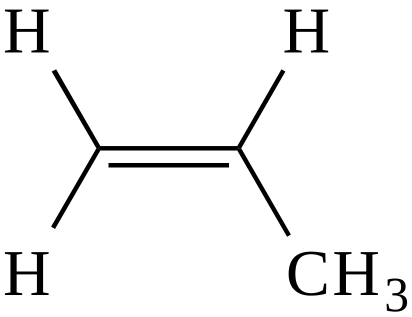


* In conformationally averaged systems.

Type of bonds…

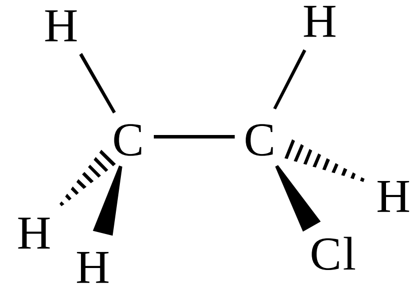
- π-bonds transmit coupling effects more effectively than σ bonds.

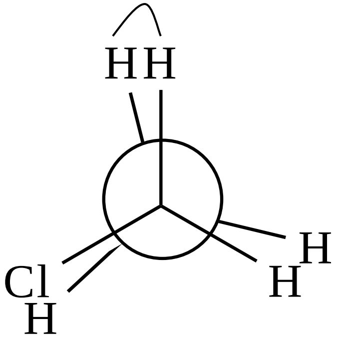


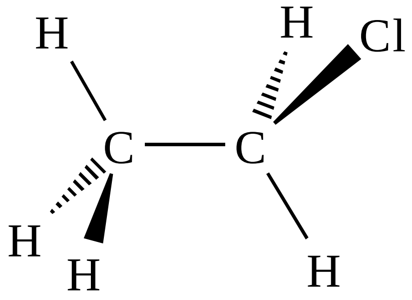


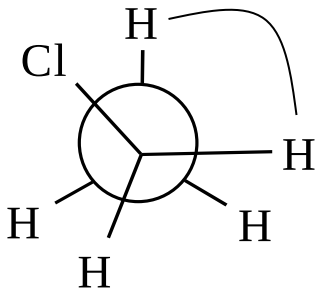
Effect of Conformations

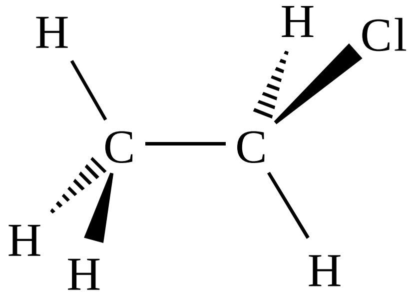
- The magnitude of vicinal couplings depends strongly on the overlap between adjacent C-H bonds.

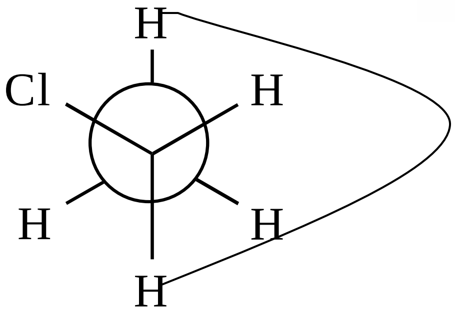


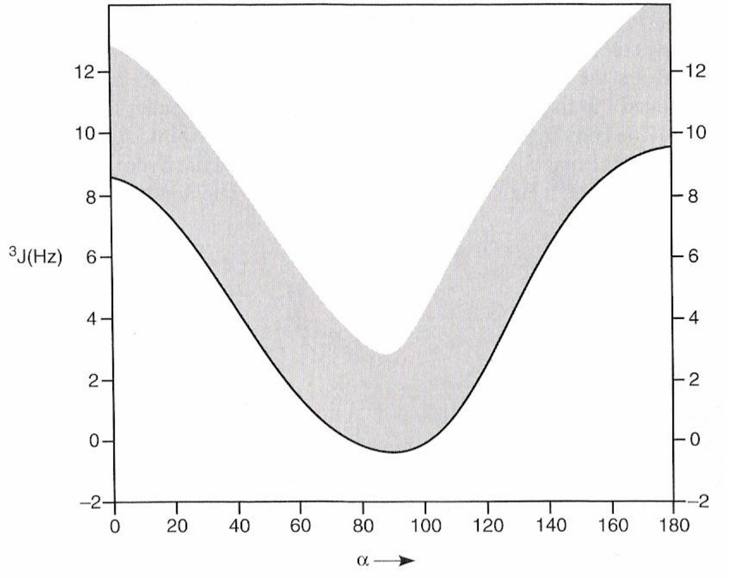






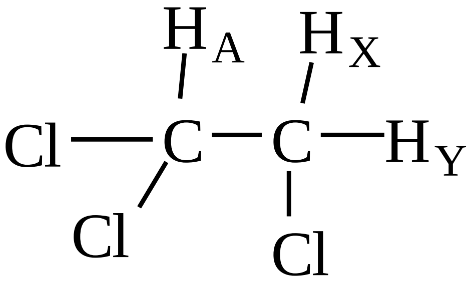






Other nuclei - spin-spin coupling (Multiplicity)

Consider the following molecule:



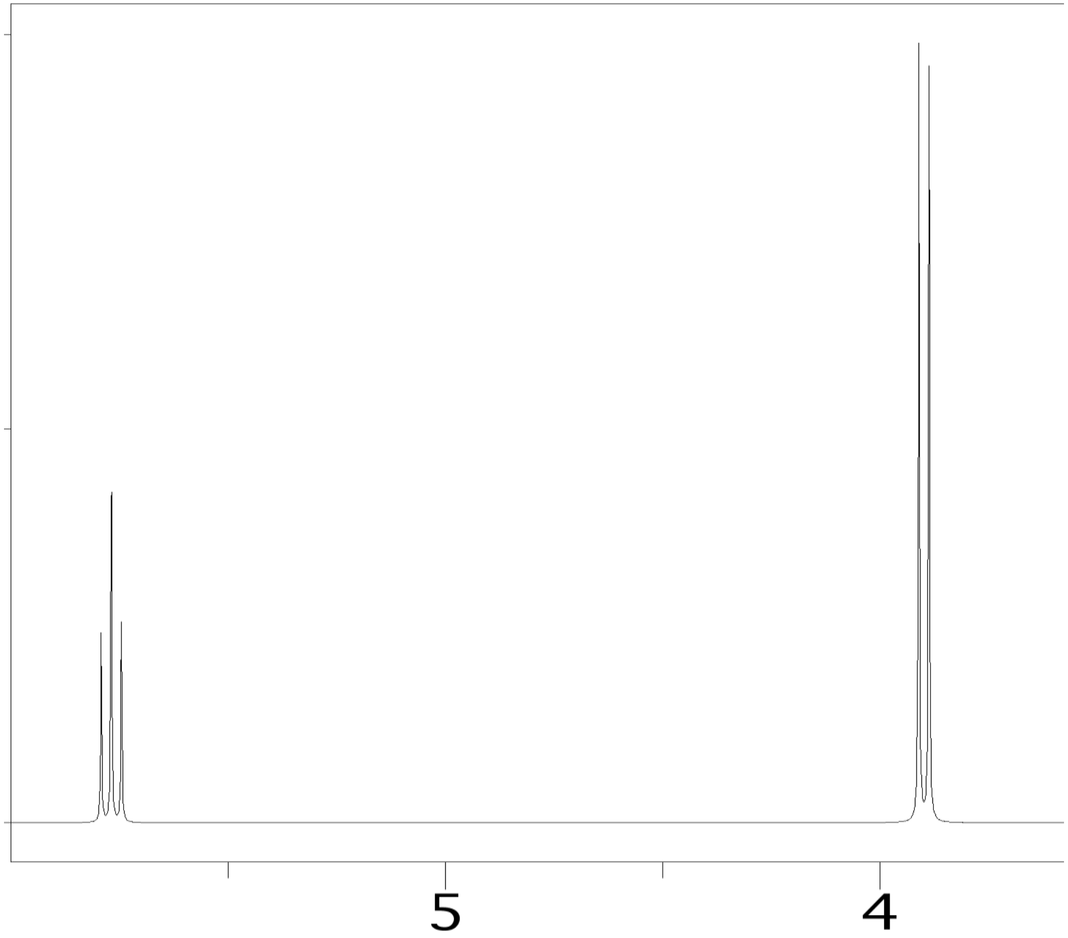
- The CH_2 has one neighbouring proton in equal proportions of the up and down spin states. This resonance will therefore appear as a …

  And H_A…

Possible spin combinations:

Other nuclei - spin-spin coupling (Multiplicity)

- Thus, H_A will appear as a three line pattern: a triplet, with peak intensities in a 1:2:1 ratio where the lines are separated by *J* Hz.
- The central line will occur at the resonance frequency of H_A.



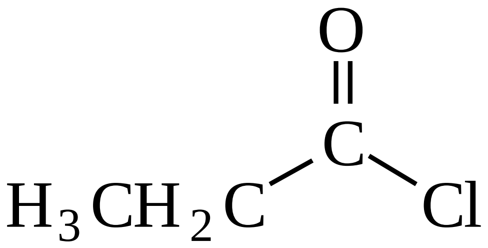
Other nuclei - spin-spin coupling (Multiplicity)

NOTE: The SIGNAL INTEGRATION tells you about the number of protons that give rise to a particular signal. MULTIPLICITY tells you about the number of …

...CHEMICALLY NON-EQUIVALENT
NEIGHBOURING NUCLEI.

- The n + 1 rule: for simple aliphatic systems, the number of lines in a given signal is n+1 where n is the no. of neighbouring protons (3 bonds away).

Other nuclei - spin-spin coupling (Multiplicity)

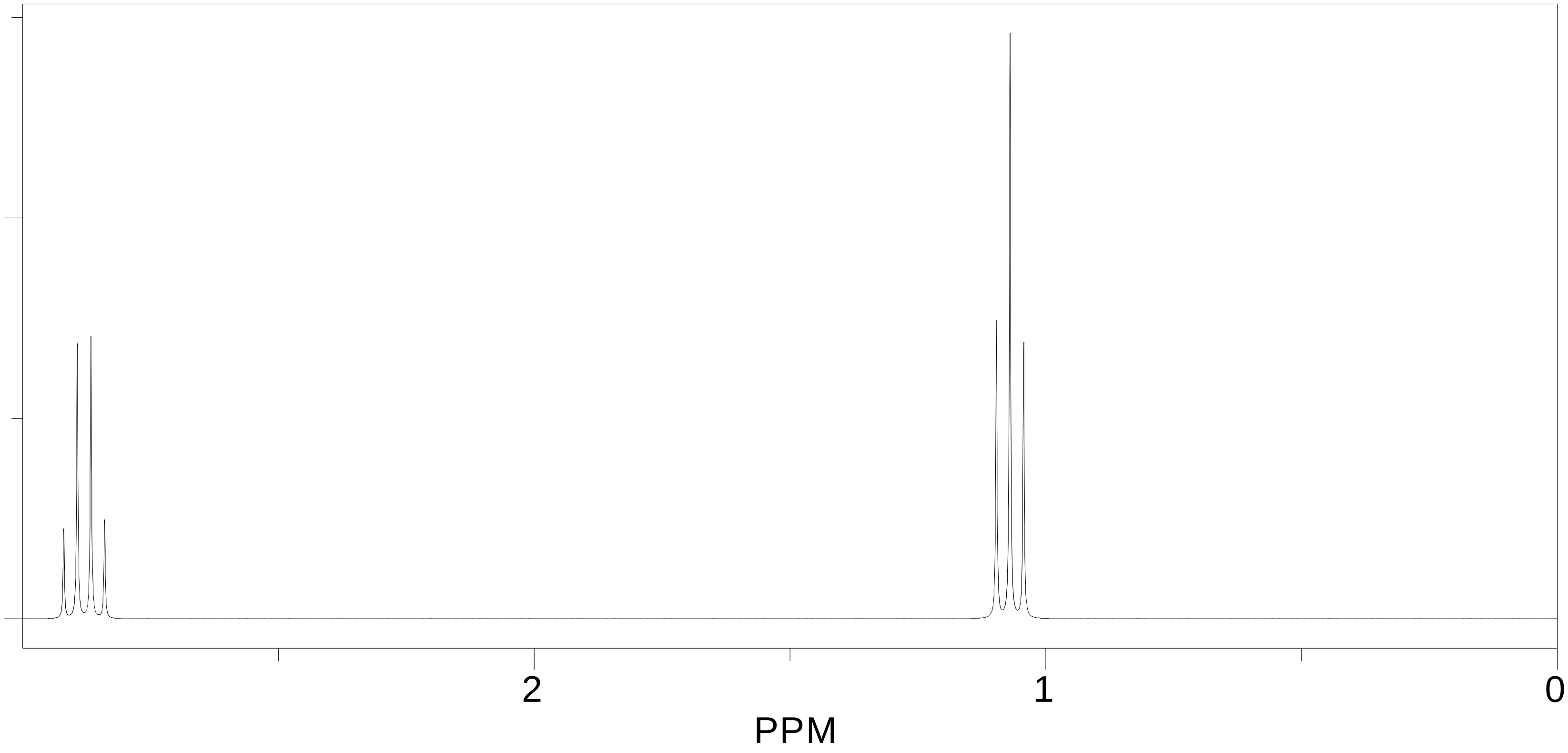


- In this molecule, the CH_3 protons will appear as a …

- The CH_2 protons have three neighbours. The spin combinations are…

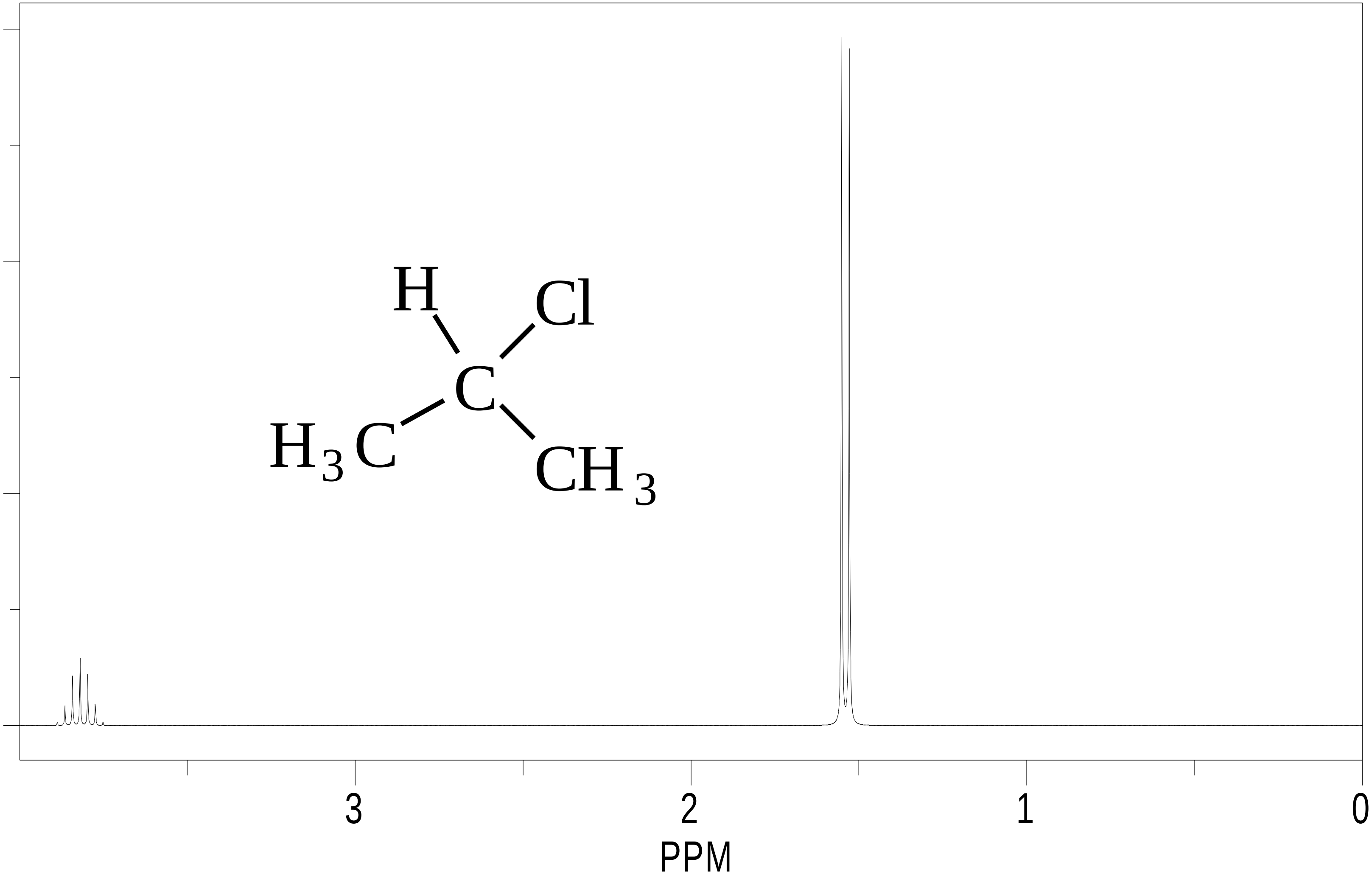
Other nuclei - spin-spin coupling (Multiplicity)

- The combination of a 2 proton quartet and a three proton triplet is characteristic of the presence of an ethyl group.



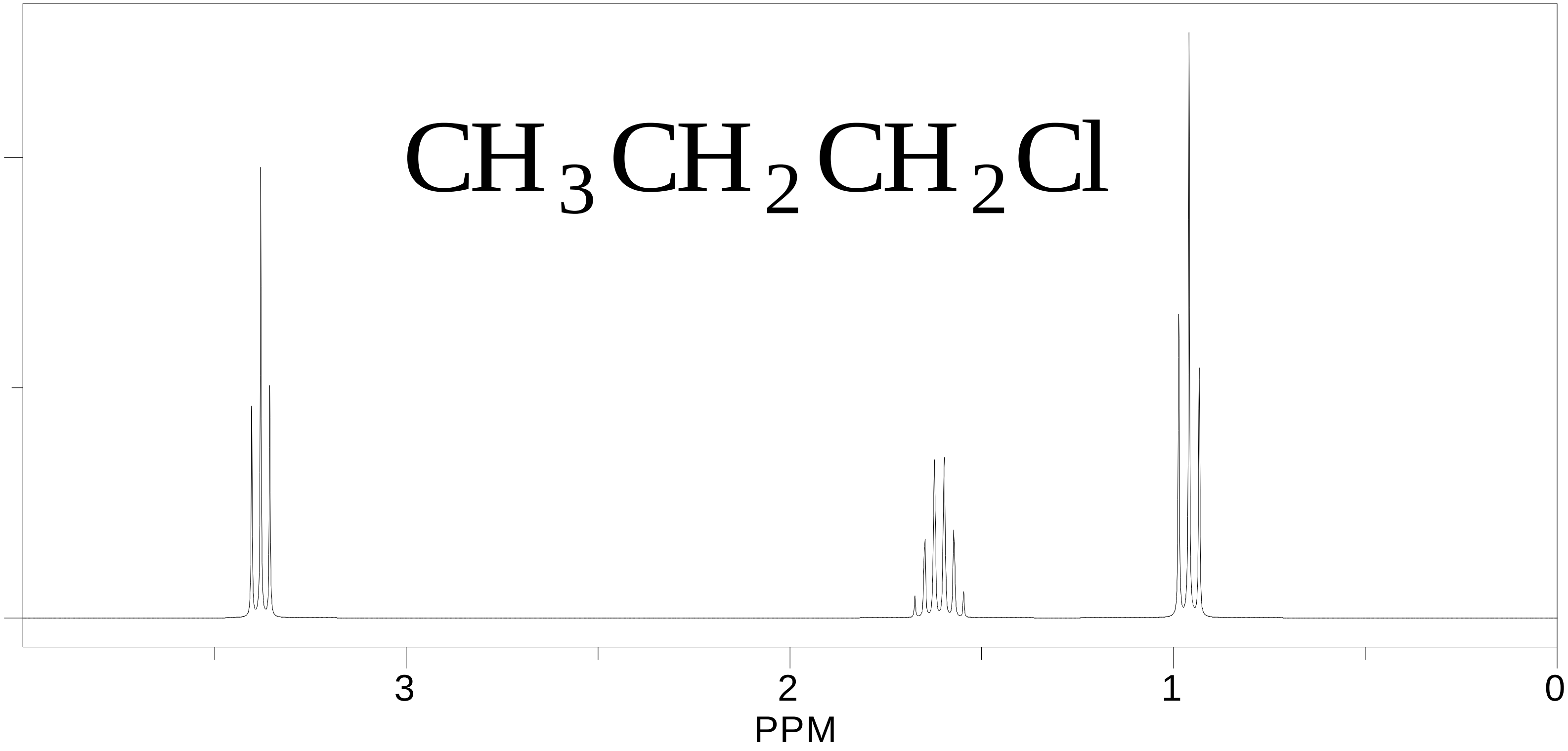
Other nuclei - spin-spin coupling (Multiplicity)

- The isopropyl group.



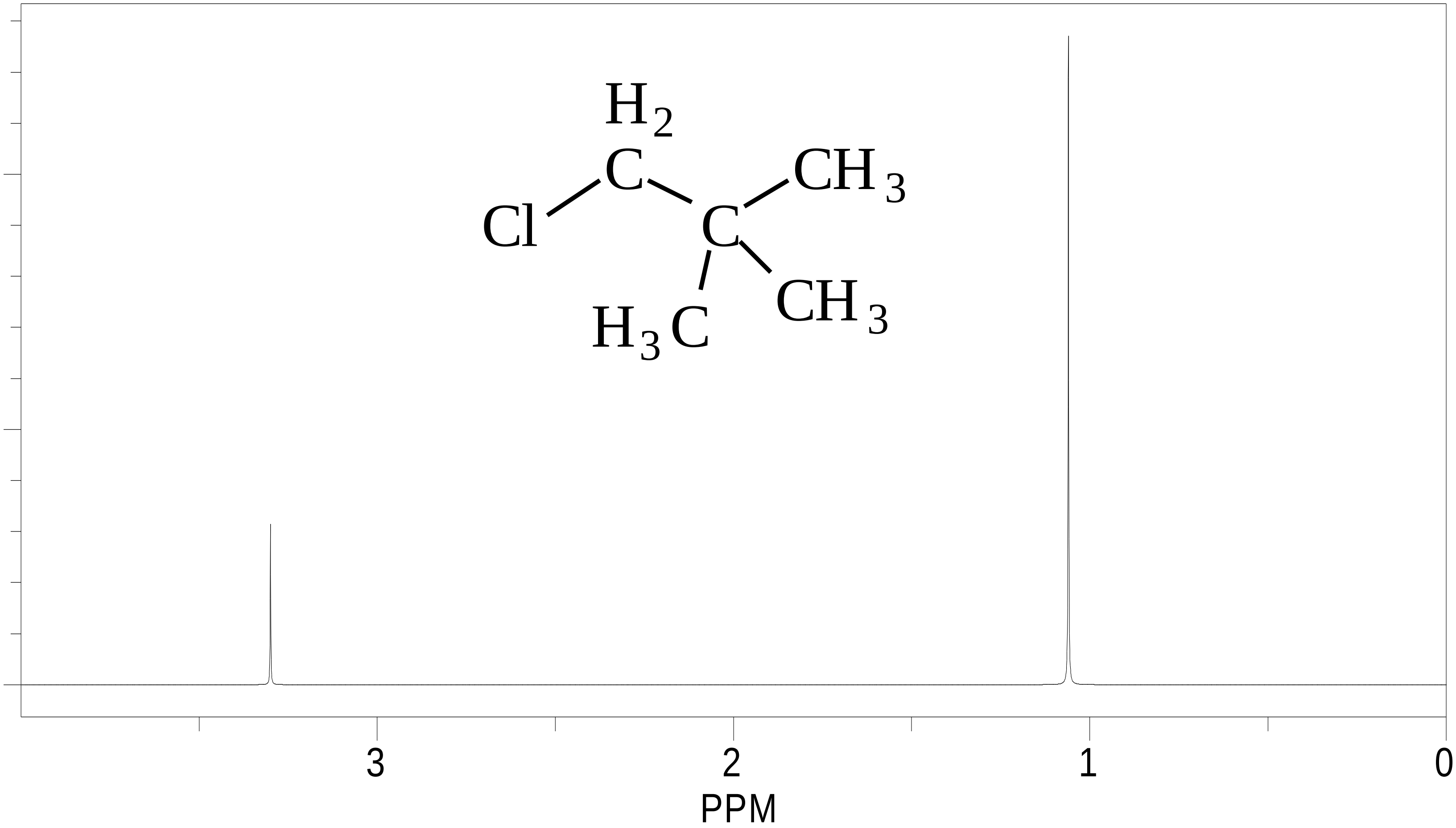
Other nuclei - spin-spin coupling (Multiplicity)

- The n-propyl group.



Other nuclei - spin-spin coupling (Multiplicity)

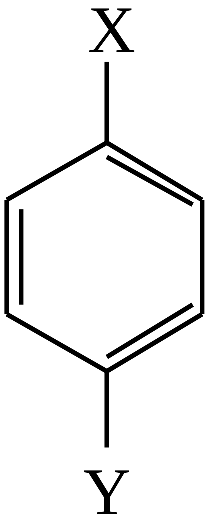
- The t-butyl group.



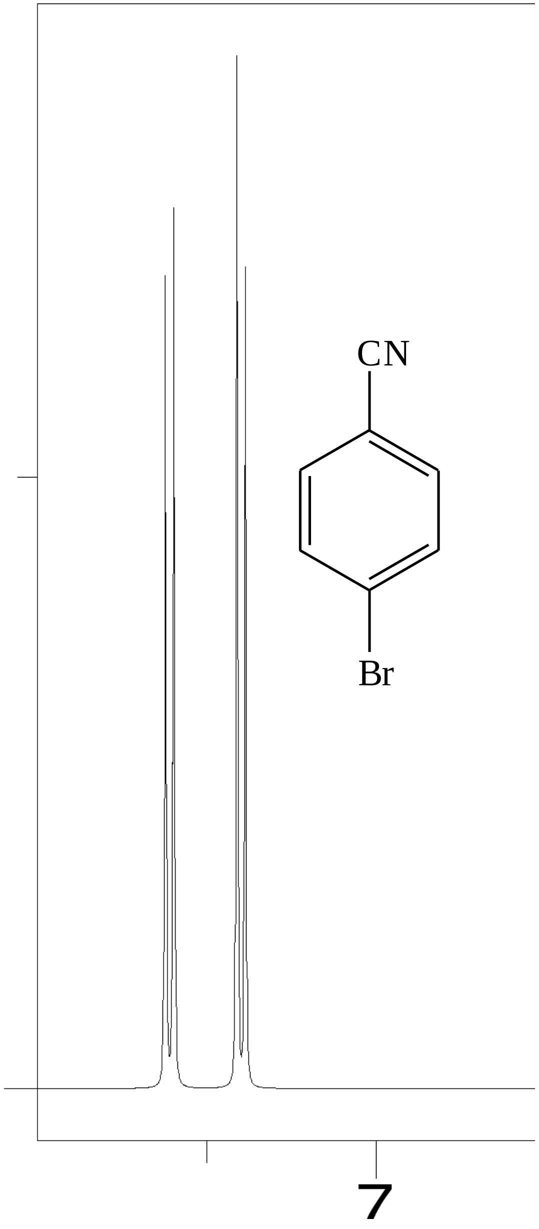
Coupling in Non n+1 Systems

- Substituted benzenes.

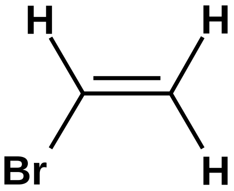
1,4

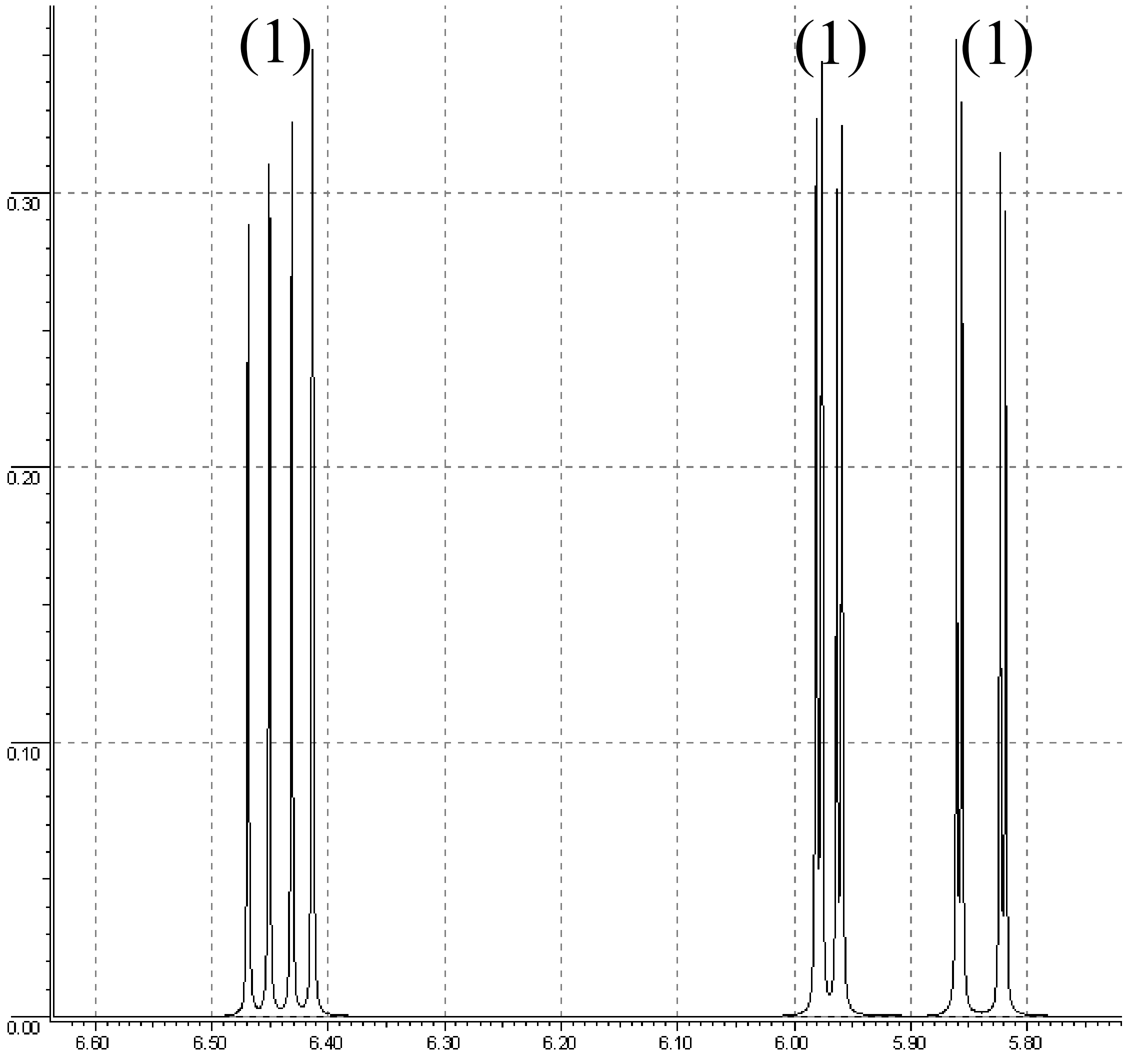


- These appear as perfectly symmetrical patterns that look like two doublets or a quartet.



The Dreaded Tree Diagram

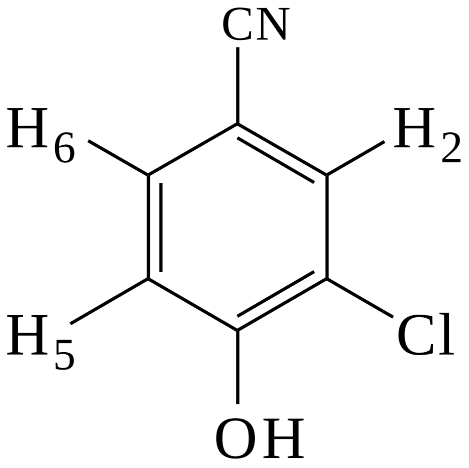




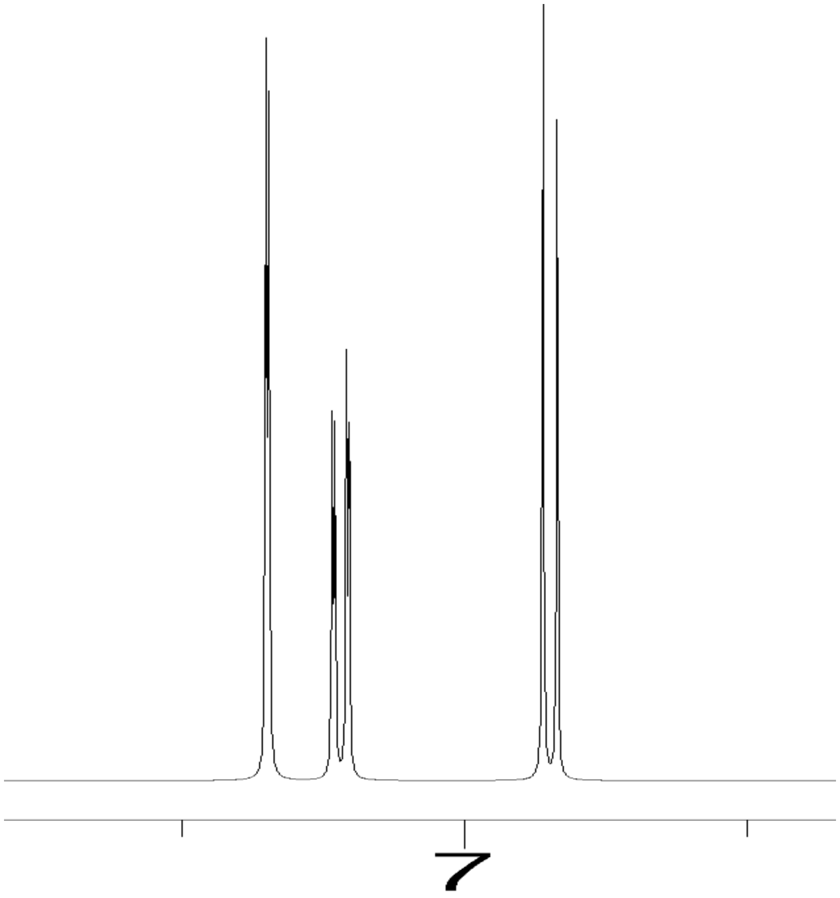
δ (ppm)

The Dreaded Tree Diagram

- 1,2,4- trisubstituted systems:

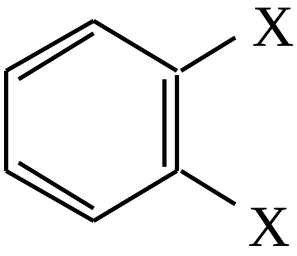


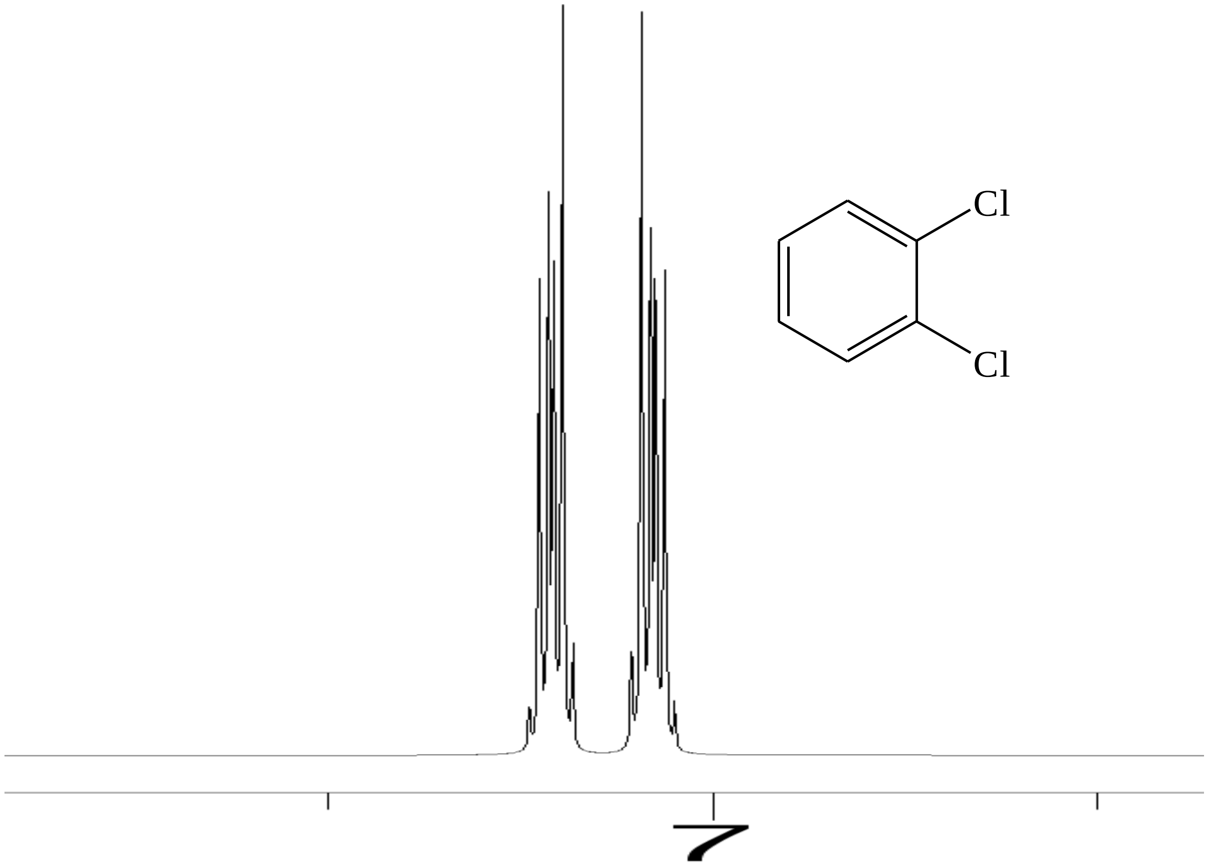
$J_{5,6}$ = 6 Hz
$J_{2,6}$ = 2 Hz
$J_{2,5}$ = 0 Hz



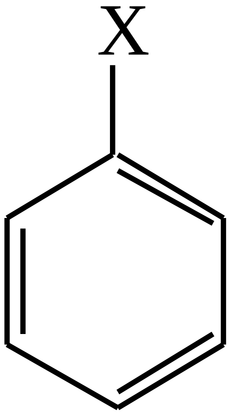
Symmetrical 1,2 Disubstituted Benzenes

- These appear as a perfectly symmetrical pattern with a lot of fine structure …





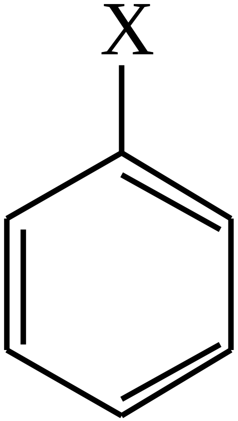
Monosubstituted Benzenes

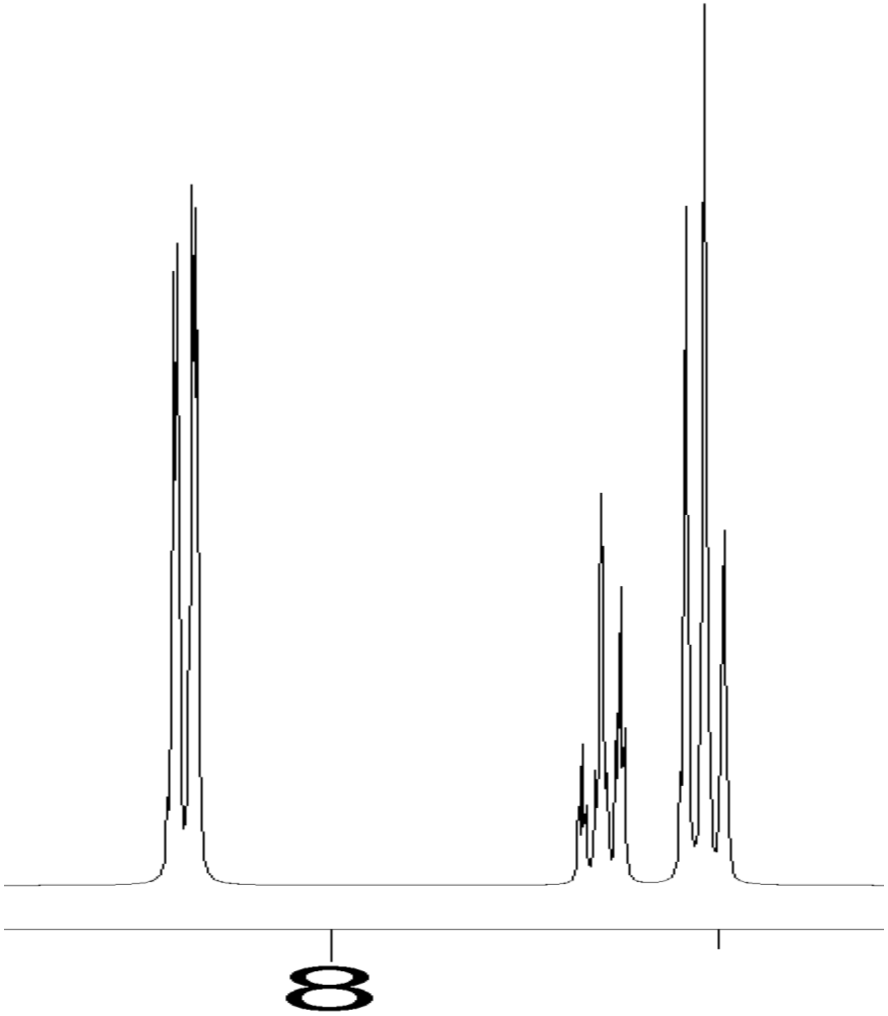


- If the substituent is an alkyl group or halogen, then all five protons tend to show up in the same place as either a singlet or a somewhat broad singlet.

Monosubstituted Benzenes

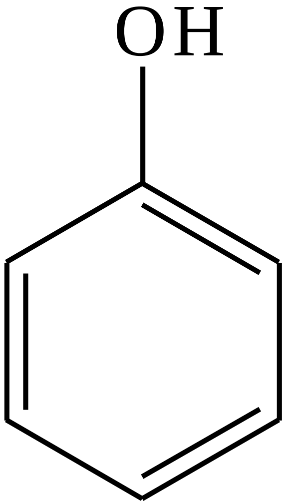
- If X is a strong electron-withdrawing group (carbonyl, nitro, sulfonic acid) then the ortho and para protons will be pulled downfield.

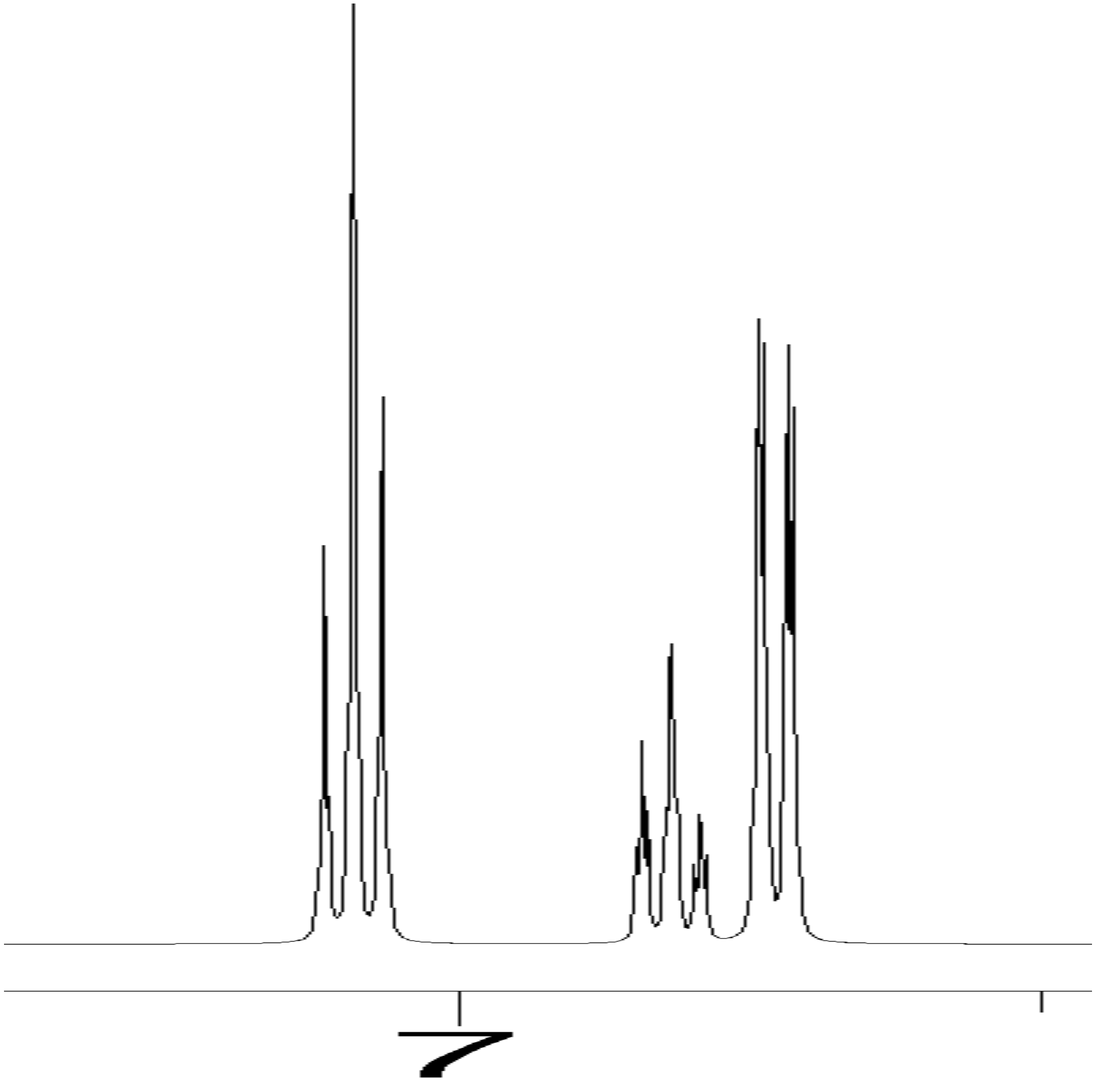




Monosubstituted Benzenes

- If X is a strong electron-donating group (OH, OR, NH_2) then the ortho and para protons are pushed upfield.



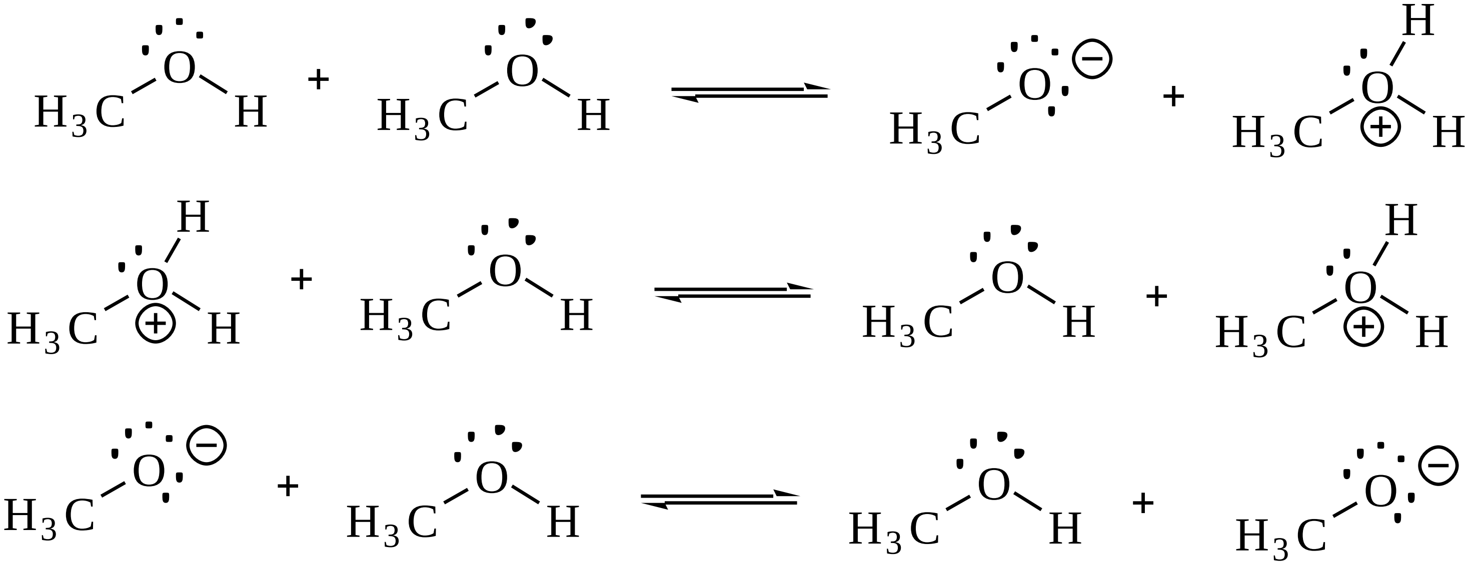


Chemical Exchange Processes - Protons Attached to O and N.

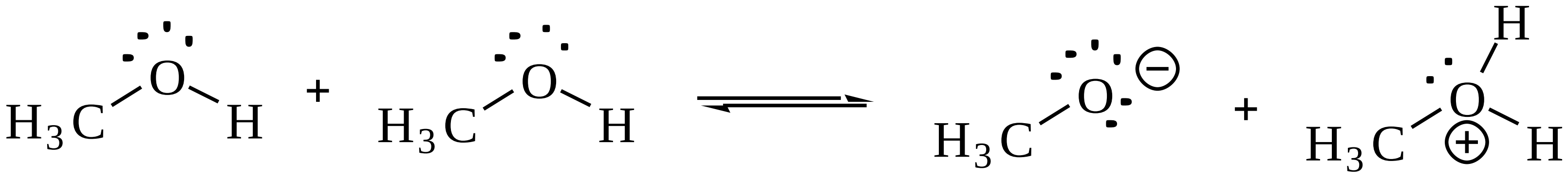
- (Alcohols, phenols, carboxylic acids, amines - but not amides)

- Unlike most spectroscopic methods, the acquisition of signal in NMR spectroscopy takes about three seconds (proton).

- In that time, protons attached to O or N can be transferred from one molecule to another via the autoionization process…



Chemical Exchange Processes - Protons Attached to O and N.



- If the rate of exchange is slow compared to the timescale of the NMR experiment (i.e. three seconds) then the spectrum is that expected of CH_3OH. Under these conditions, vicinal OH:CH coupling is observed. This is rarely the case.

- If the rate of exchange is comparable to the NMR timescale, then one observes the exchanging proton in a *range* of environments and at a range of chemical shift postions.

- Under these conditions, the OH peak is broad and coupling is not observed…

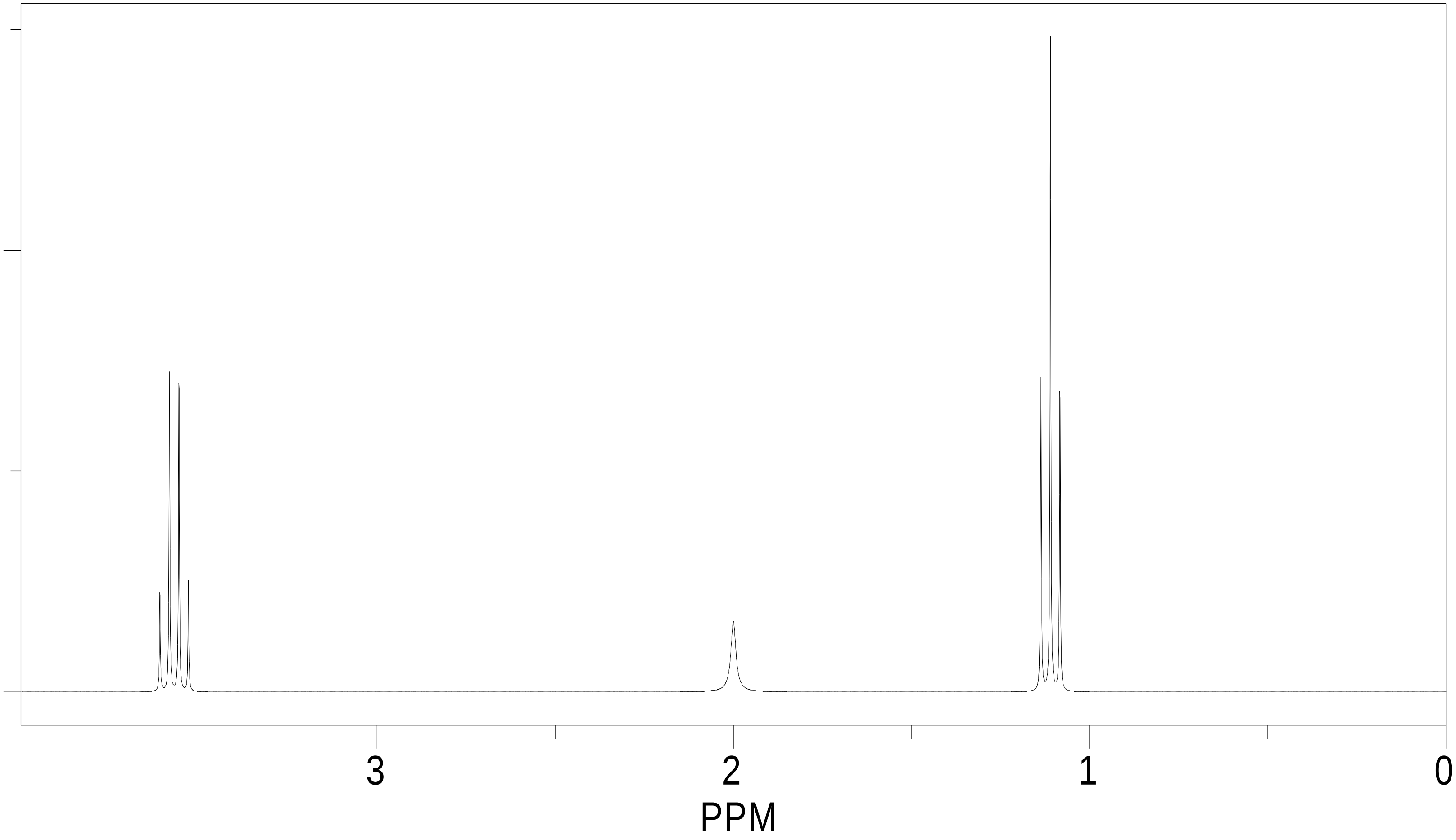
Chemical Exchange Processes - Protons Attached to O and N.

- The rate of exchange is catalyzed by acids and bases, depends on solvent, temperature, concentration, purity, and lunar phase.

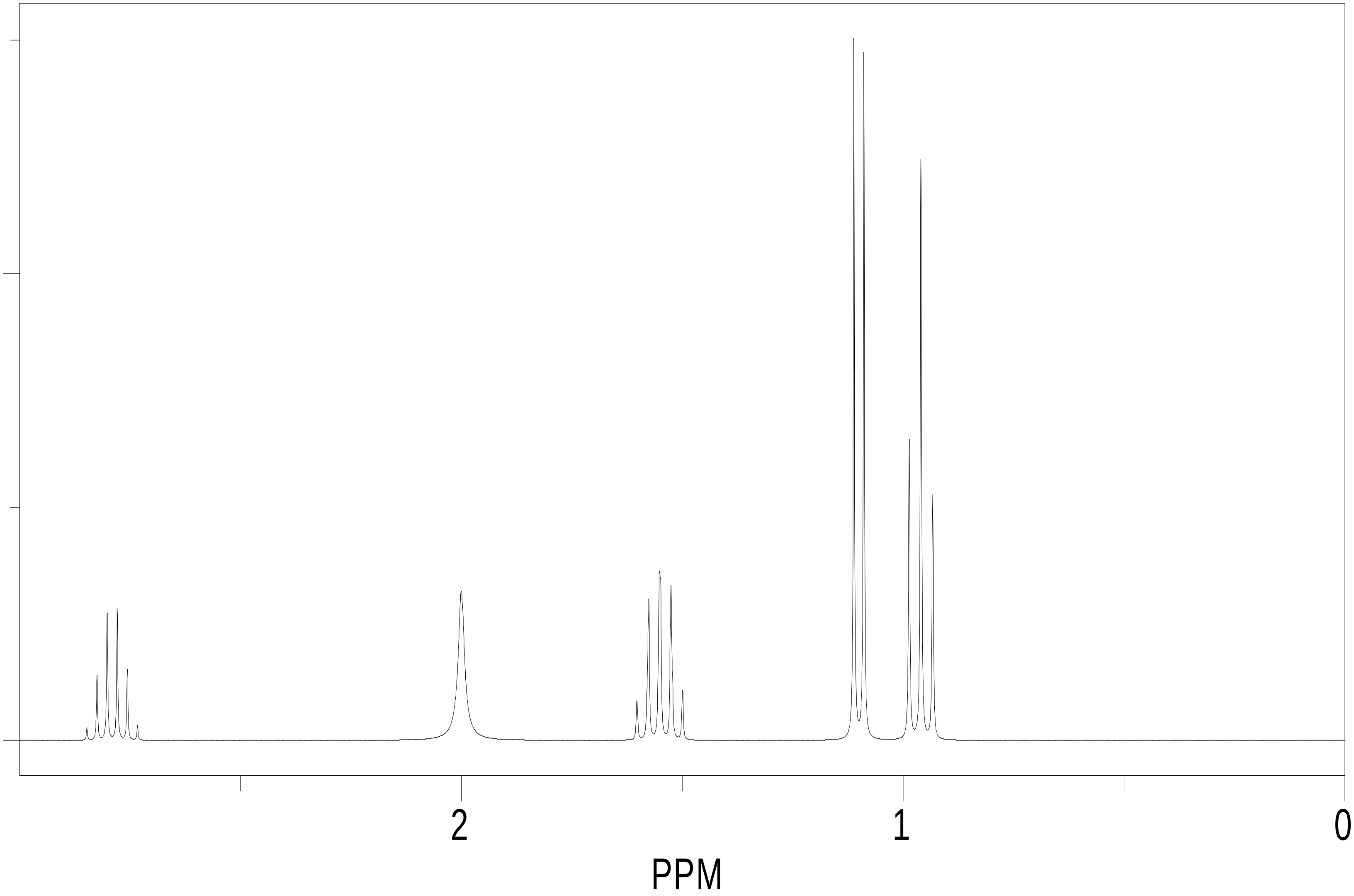
Exchangeable protons…

- do not couple
- have variable shift positions
- are observed as broad peaks
- exchange with D_2O

Chemical Exchange Processes - Protons Attached to O and N.



Chemical Exchange Processes - Protons Attached to O and N.



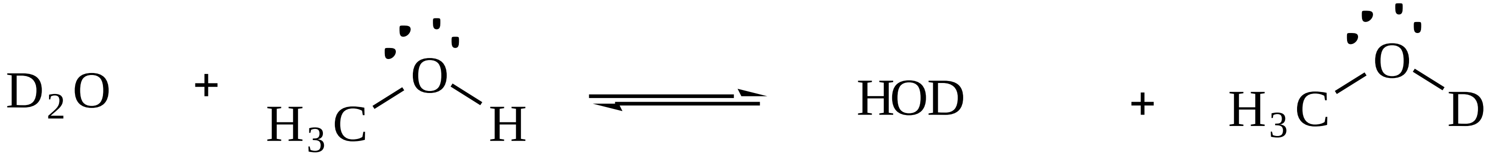
Chemical Exchange Processes - Protons Attached to O and N.

- Occasionally, carboxylic acid protons resonances are so broad …

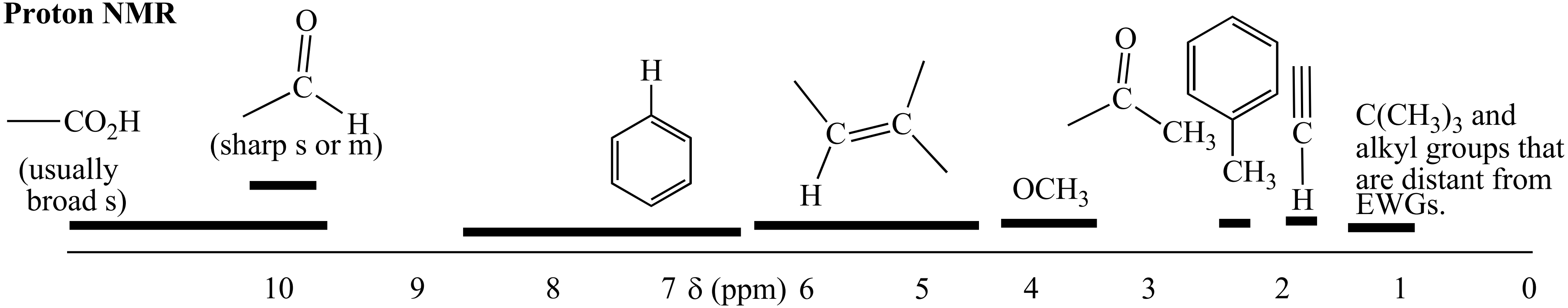
..that the only way to tell that they are there is to integrate the baseline.

D_2O exchange

- Exchangeable protons on a molecule will exchange with exchangeable protons on other molecules…



Proton NMR



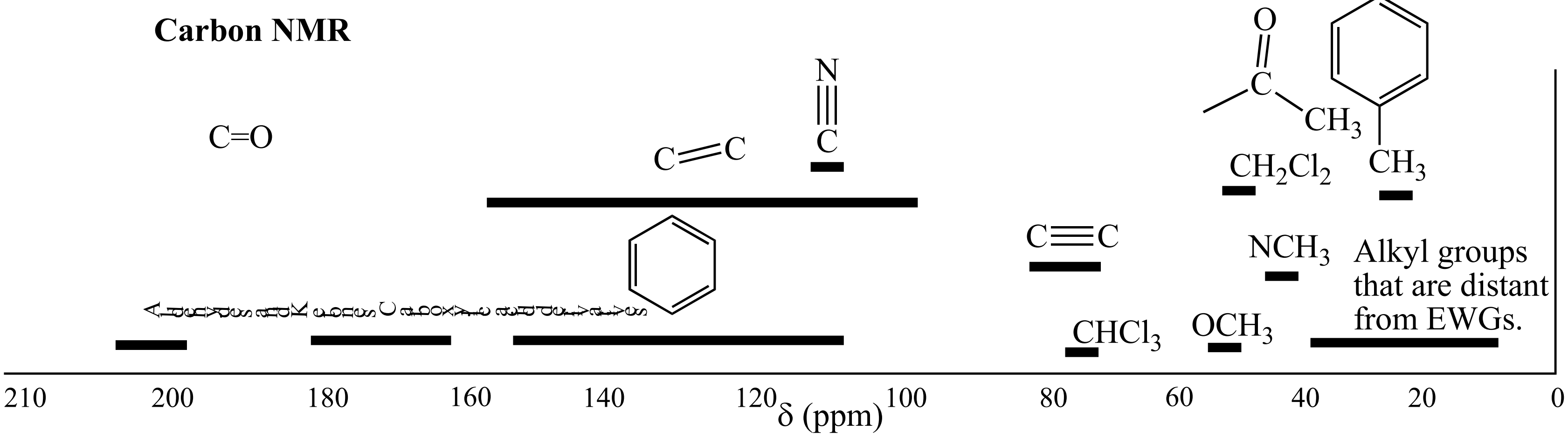
Alkyl protons cover a range of chemical shifts depending on the natrue and number of the electron-withdrawing groups (EWGs) that are nearby. Methyl groups are found between 0.9 and 4.2 ppm (pentane to C**H**$_3$OCOAr). Methylene (CH$_2$) groups are found between 1.2 (pentane) and 5.2 ppm (CH$_2$Cl$_2$). Methine (CH) groups range between 1.5 ppm ((CH$_3$)$_3$C**H**) to 5.6 ppm (PhC**H**(OCH$_3$)$_2$) to 7.27 ppm (CHCl$_3$) depending on the three substituents.

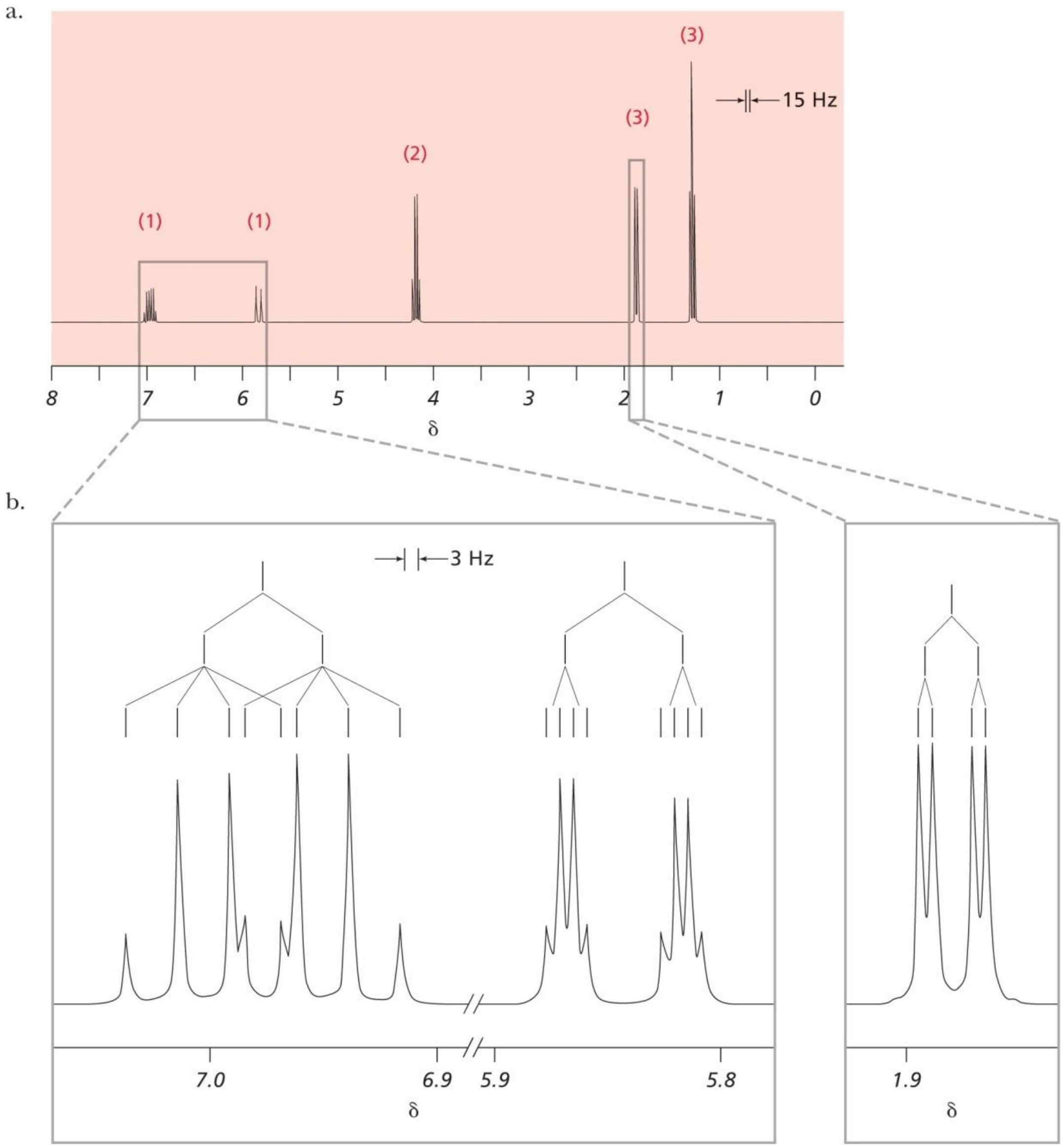
IF YOUR SPECTRUM HAS A BROAD PEAK then it is almost certinaly an NH, NH$_2$ or OH gropu and not CH. These peaks can occur anywhere between 1.5-14 ppm and vary even from sample to sampe of the same compound! Only carboxylic acids are somewhat consistent at ~10 ppm.

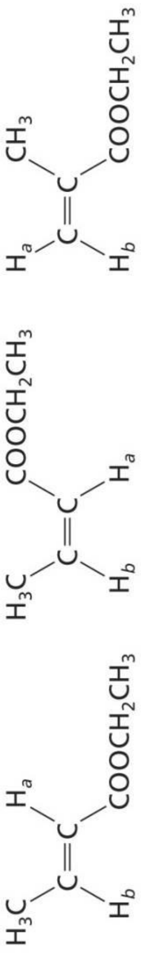
Ethynyl (vinyl C=C**H**) protons are usually found at 5-6.5 ppm. They are found in the upfield portion of this range if an O or N atom is directly attached (beta to H, i.e. ROCH=C**H**) and downfield in this range if a carbonyl, nitro or CN group is attached to the double bond (i.e. O=C-C=C**H**).

Aromatic protons (PhH) are usually found around 7-7.5 ppm. They may be shielded upfield of this range (as far as 6.5) by lone-pair donating groups (OH and NH - strong o/p directing ring activators)or downfield of this range (7.5-8.5 ppm) by electron-withdrawing groups(C=O, NO$_2$, SO$_3$H i.e. strong meta-directing deactivators).

Carbon NMR







$J(CH_3, H_a)$	2	2	2
$J(CH_3, H_b)$	7	7	2
$J(H_a, H_b)$	15	7	2

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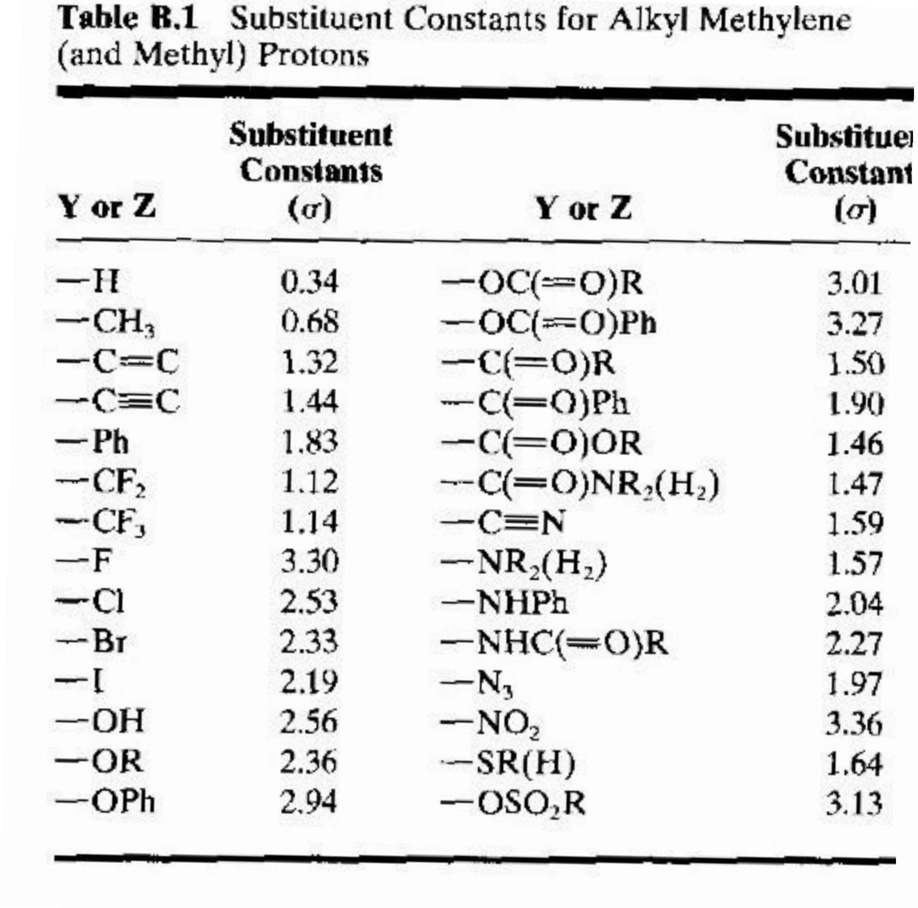


Table B.1 Substituent Constants for Alkyl Methylene (and Methyl) Protons

Y or Z	Substituent Constants (σ)	Y or Z	Substitue Constant (σ)
$-H$	0.34	$-OC(=O)R$	3.01
$-CH_3$	0.68	$-OC(=O)Ph$	3.27
$-C=C$	1.32	$-C(=O)R$	1.50
$-C\equiv C$	1.44	$-C(=O)Ph$	1.90
$-Ph$	1.83	$-C(=O)OR$	1.46
$-CF_2$	1.12	$-C(=O)NR_2(H_2)$	1.47
$-CF_3$	1.14	$-C\equiv N$	1.59
$-F$	3.30	$-NR_2(H_2)$	1.57
$-Cl$	2.53	$-NHPh$	2.04
$-Br$	2.33	$-NHC(=O)R$	2.27
$-I$	2.19	$-N_3$	1.97
$-OH$	2.56	$-NO_2$	3.36
$-OR$	2.36	$-SR(H)$	1.64
$-OPh$	2.94	$-OSO_2R$	3.13

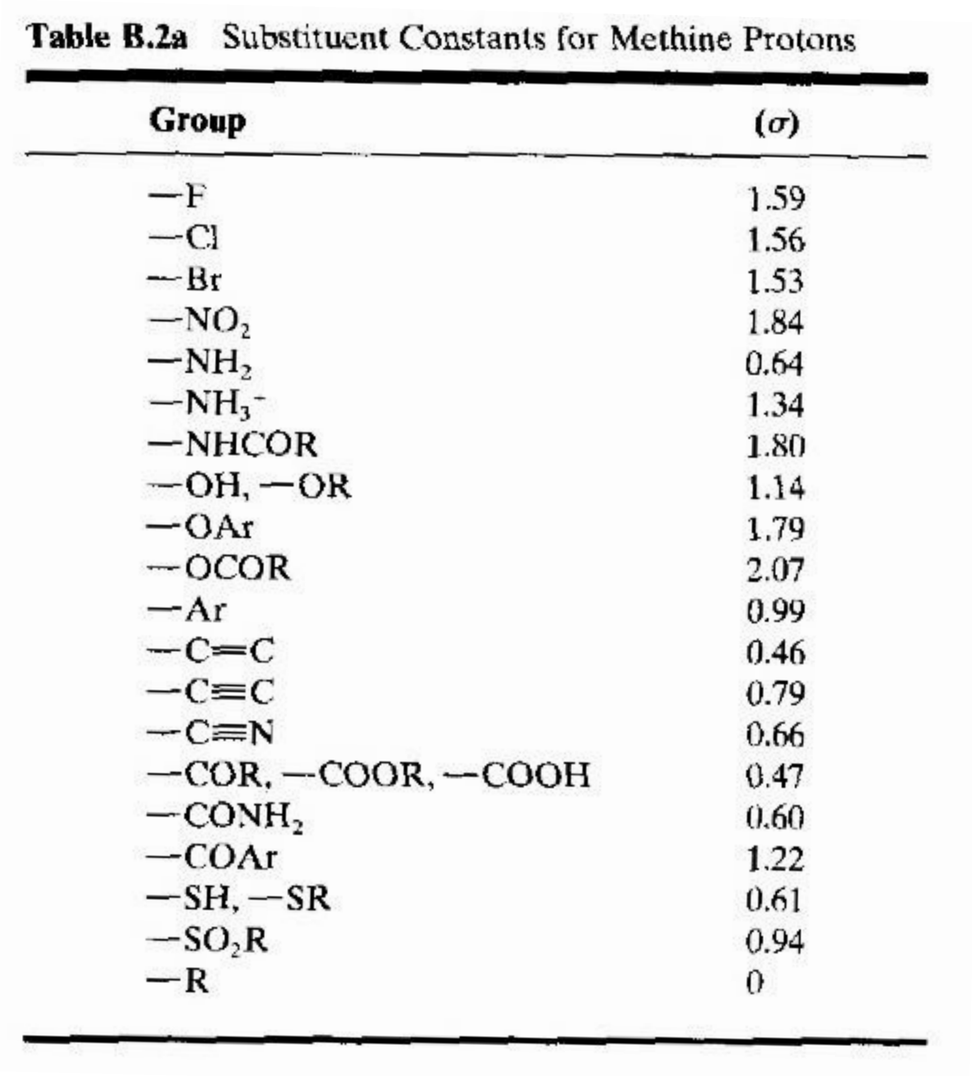
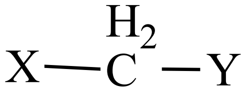


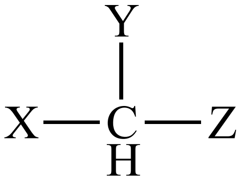
Table B.2a Substituent Constants for Methine Protons

Group	(σ)
$-F$	1.59
$-Cl$	1.56
$-Br$	1.53
$-NO_2$	1.84
$-NH_2$	0.64
$-NH_3^+$	1.34
$-NHCOR$	1.80
$-OH$, $-OR$	1.14
$-OAr$	1.79
$-OCOR$	2.07
$-Ar$	0.99
$-C=C$	0.46
$-C\equiv C$	0.79
$-C\equiv N$	0.66
$-COR$, $-COOR$, $-COOH$	0.47
$-CONH_2$	0.60
$-COAr$	1.22
$-SH$, $-SR$	0.61
$-SO_2R$	0.94
$-R$	0



$X-\overset{H_2}{C}-Y$

$$\delta = 0.23 + \delta_X + \delta_Y$$

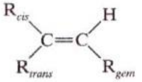


$X-\underset{H}{\overset{Y}{C}}-Z$

$$\delta = 2.50 + \delta_X + \delta_Y + \delta_Z$$

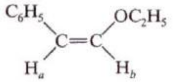
Appendix D Chemical Shifts in Unsaturated and Aromatic Systems

(See Table D.1)



$$\delta_H = 5.25 + Z_{gem} + Z_{cis} + Z_{trans}$$

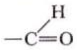
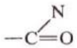
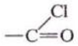
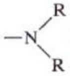
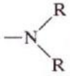
For example, the chemical shifts of the alkene protons in



are calculated:

H_a	$C_6H_{5\,gem}$	1.35	5.25
	OR_{trans}	$-\underline{1.28}$	$\underline{0.07}$
		0.07	δ 5.32
H_b	OR_{gem}	1.18	5.25
	$C_6H_{5\,trans}$	$-\underline{0.10}$	$\underline{1.08}$
		1.08	δ 6.33

Table D.1 Substituent Constants *(Z)* for Chemical Shifts of Substituted Ethylenes

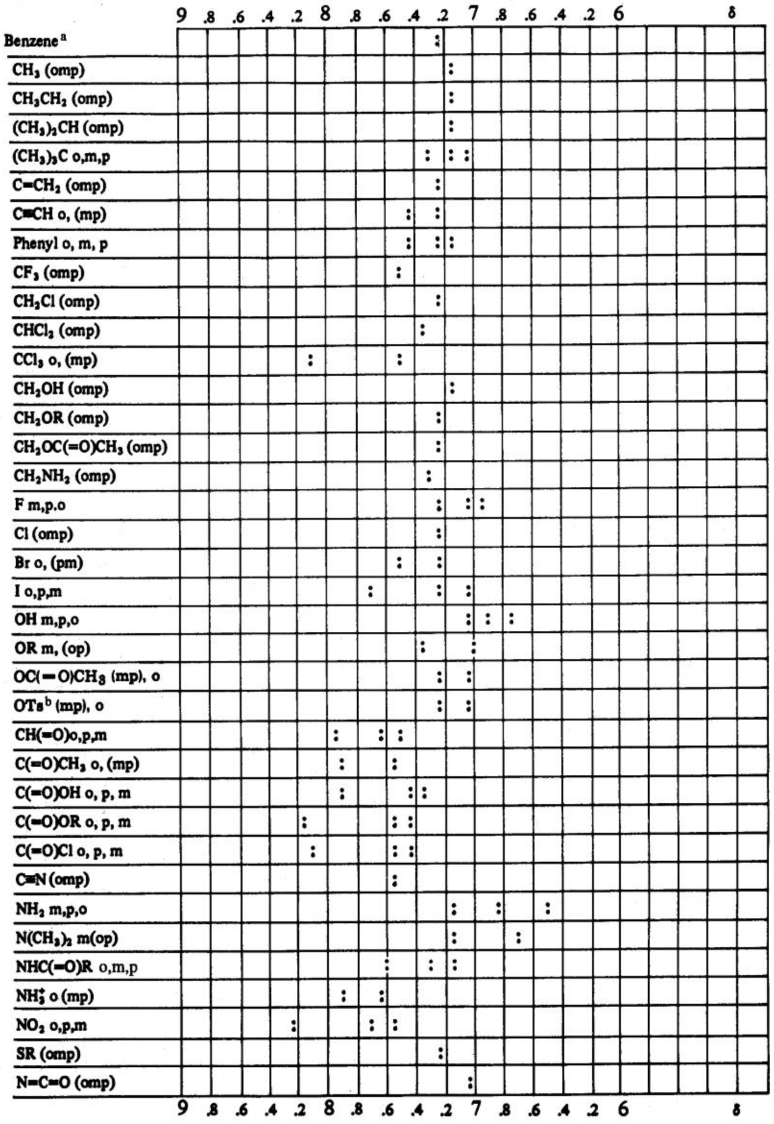
		Z				Z	
Substituent R	**gem**	**cis**	**trans**	**Substituent R**	**gem**	**cis**	**trans**
—H	0	0	0				
—Alkyl	0.44	−0.26	−0.29	 $-\overset{H}{C}{=}O$	1.03	0.97	1.21
—Alkyl-ring[a]	0.71	−0.33	−0.30				
—CH_2O, —CH_2I	0.67	−0.02	−0.07				
—CH_2S	0.53	−0.15	−0.15	 $-\overset{N}{C}{=}O$	1.37	0.93	0.35
—CH_2Cl, —CH_2Br	0.72	0.12	0.07				
—CH_2N	0.66	−0.05	−0.23	 $-\overset{Cl}{C}{=}O$	1.10	1.41	0.99
—C≡C	0.50	0.35	0.10				
—C≡N	0.23	0.78	0.58	—OR, R:aliph	1.18	−1.06	−1.28
—C=C	0.98	−0.04	−0.21	—OR, R:conj[b]	1.14	−0.65	−1.05
—C=C conj[b]	1.26	0.08	−0.01	—OCOR	2.09	−0.40	−0.67
—C=O	1.10	1.13	0.81	—Aromatic	1.35	0.37	−0.10
—C=O conj[b]	1.06	1.01	0.95	—Cl	1.00	0.19	0.03
—COOH	1.00	1.35	0.74	—Br	1.04	0.40	0.55
—COOH conj[b]	0.69	0.97	0.39	 $-N{<}^{R}_{R}$ R:aliph	0.69	−1.19	−1.31
—COOR	0.84	1.15	0.56	 $-N{<}^{R}_{R}$ R:conj[b]	2.30	−0.73	−0.81
—COOR conj[b]	0.68	1.02	0.33				
				—SR	1.00	−0.24	−0.04
				—SO_2	1.58	1.15	0.95

[a] Alkyl ring indicates that the double bond is part of the ring  .

[b] The *Z* factor for the conjugated substituent is used when either the substituent or the double bond is further conjugated with other groups.

Source: Pascual C., Meier, J., and Simon, W. (1966) *Helv. Chim. Acta,* **49,** 164.

Chart D.1. Chemical Shifts of Protons on Monosubstituted Benzene Rings



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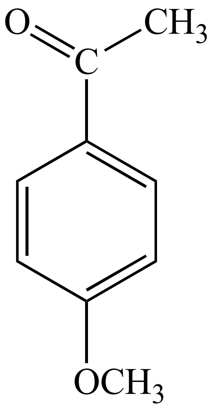
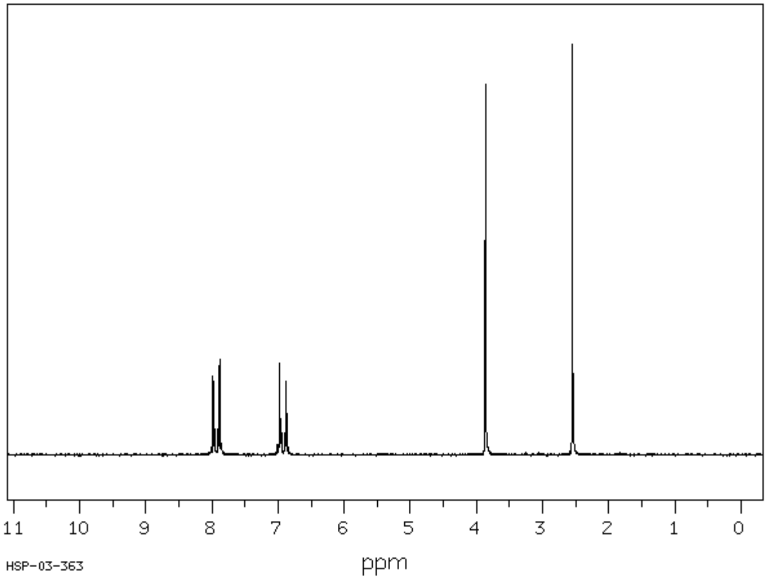
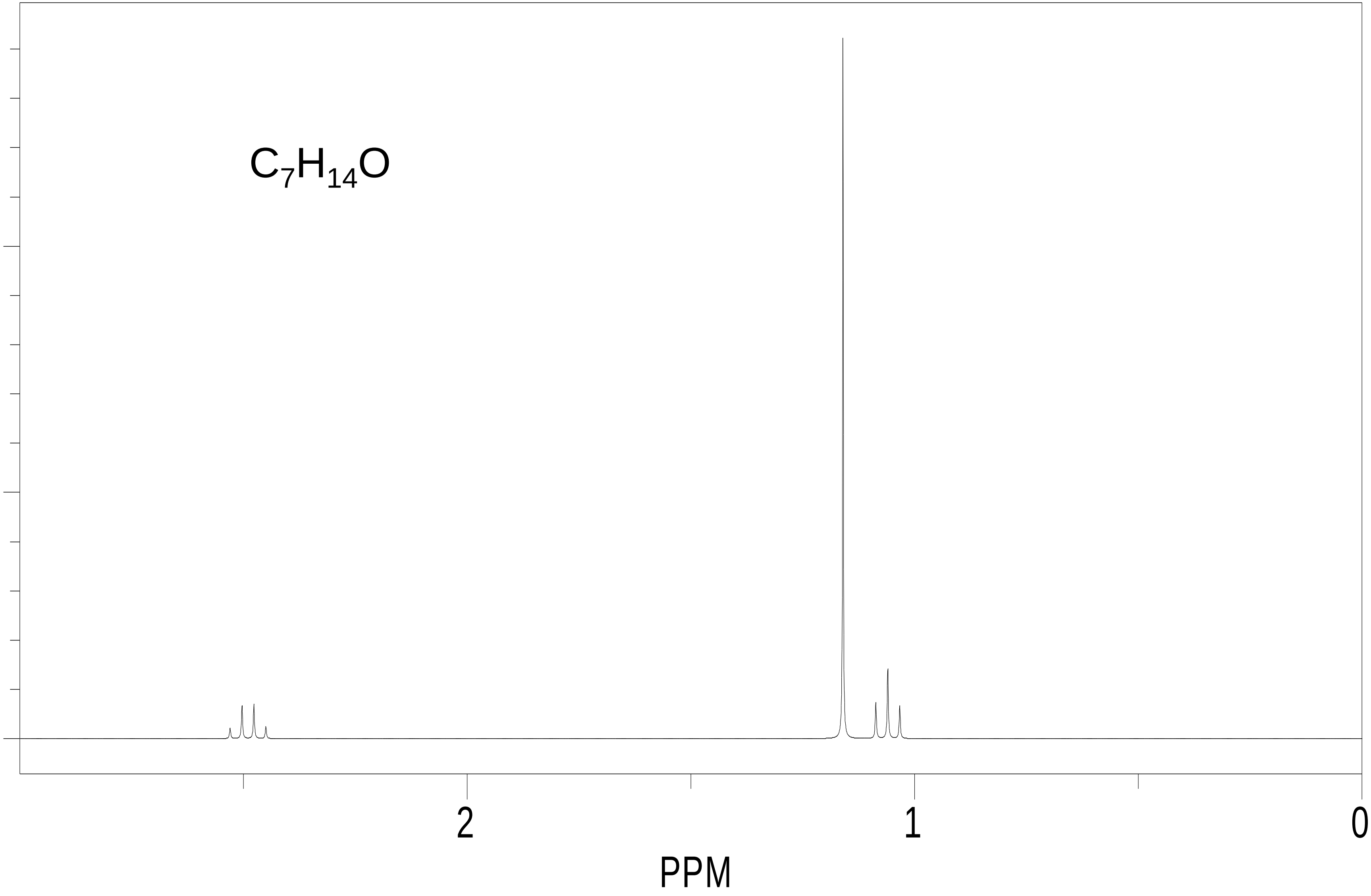
[a] The benzene ring proton is at δ 7.27, from which the shift increments are calculated as shown at the end of Section 4.7.

[b] OTS = *p*-toluenesulfonyloxy group.





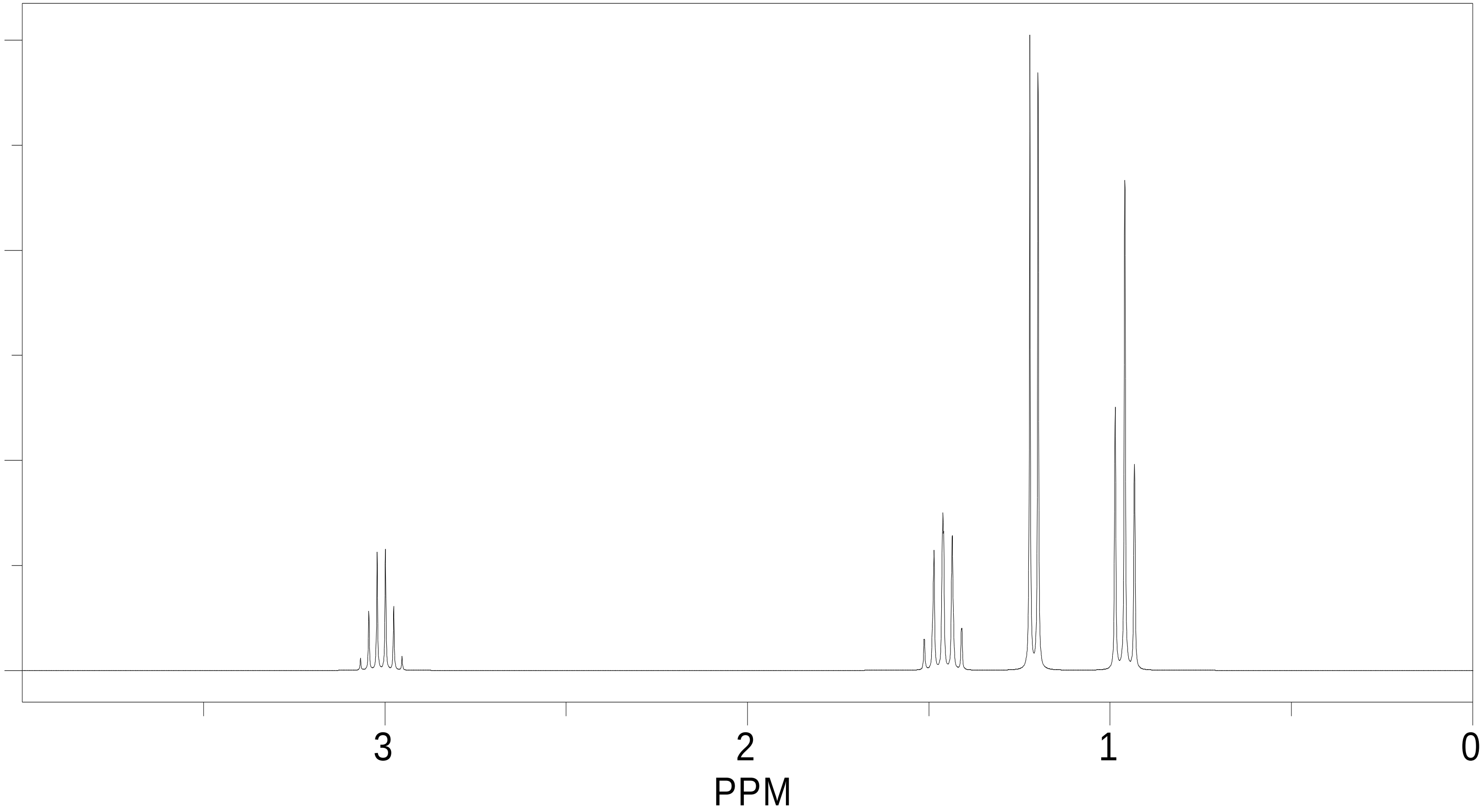
NMR Spectroscopy



Int: 2:9:3

NMR Spectroscopy

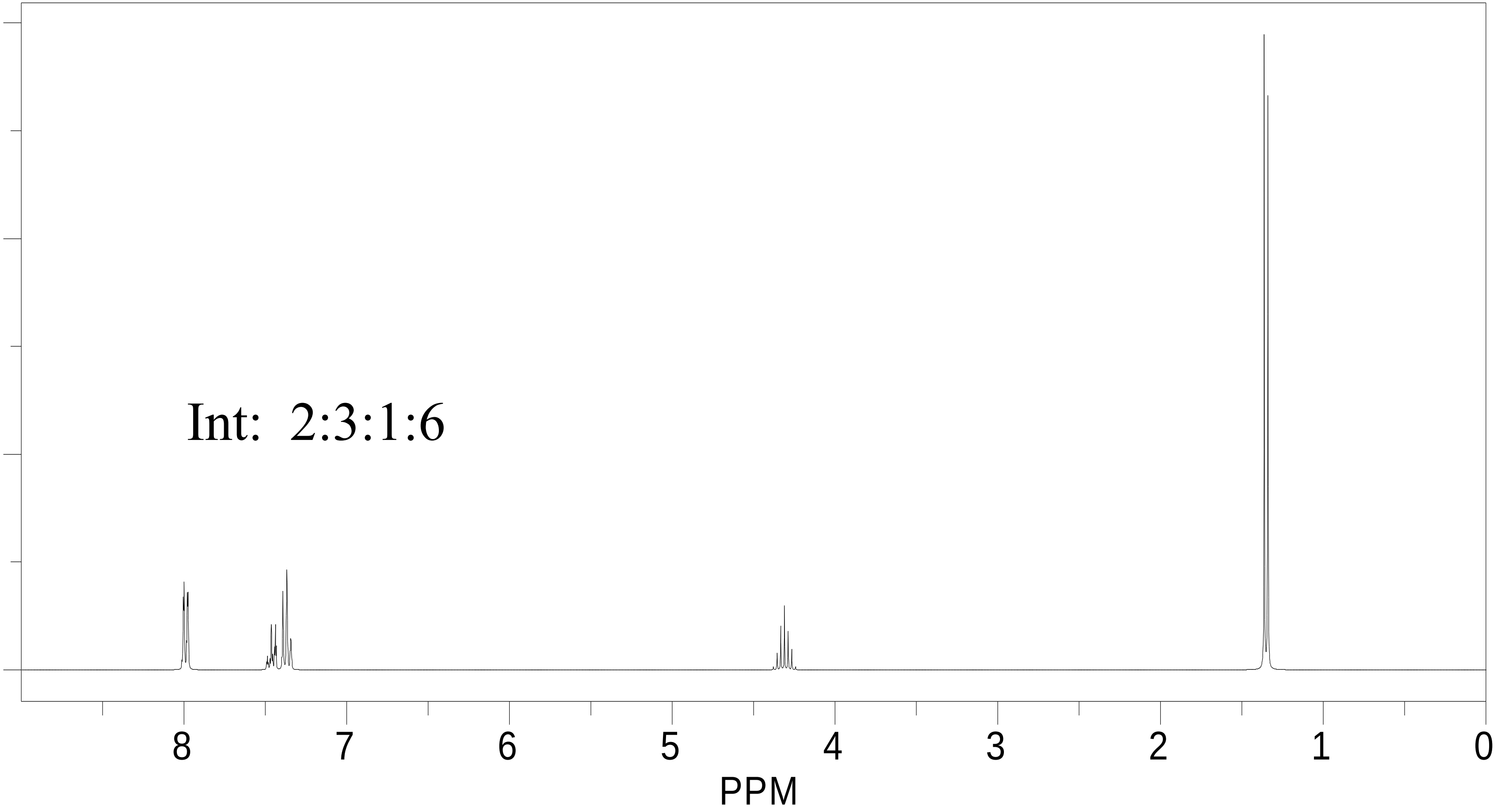
$C_8H_{18}O$



Int: 1:2:3:3

NMR Spectroscopy

$C_{10}H_{12}O_2$



^{13}C NMR Spectroscopy

- ^{12}C is spin zero ($I = 0$) so we rely on ^{13}C

Problems:

- ^{13}C is only 1% abundant ($I = ½$)
- magnetogyric ratio is ¼ that of ^{1}H

- Routine ^{13}C NMR was unavailable until the development of Fourier Transform instruments.

^{1}H and ^{13}C NMR Spectroscopy

Similarities…

- chemical shift effects are the same but over a much larger scale (spectral width is ~ 250 ppm: –10 to 240 ppm)
- scale is defined in the same way

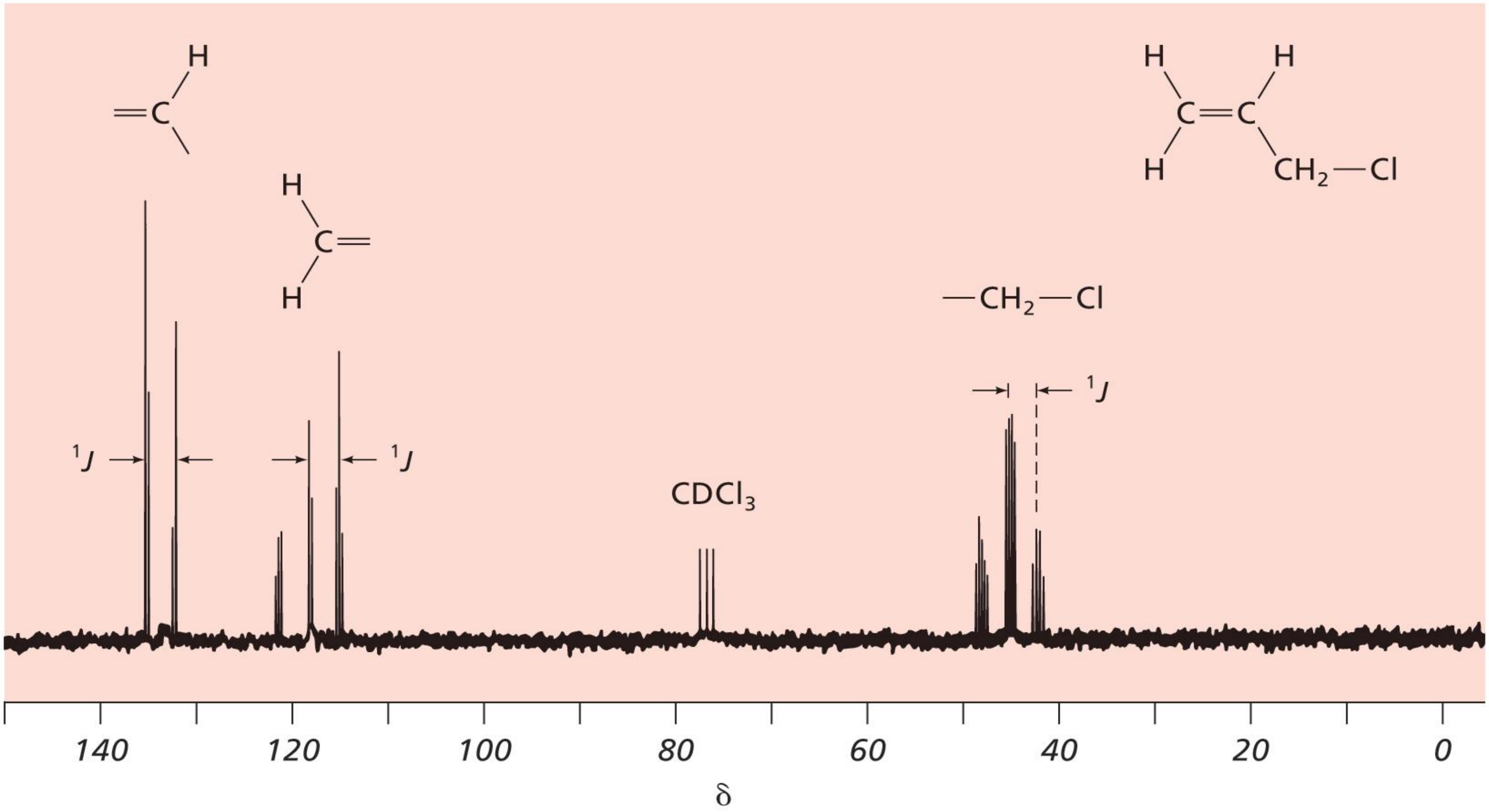
Differences…

- integrations are not valid
- ^{13}C-^{13}C coupling is not observed
- ^{13}C-^{1}H coupling is usually eliminated

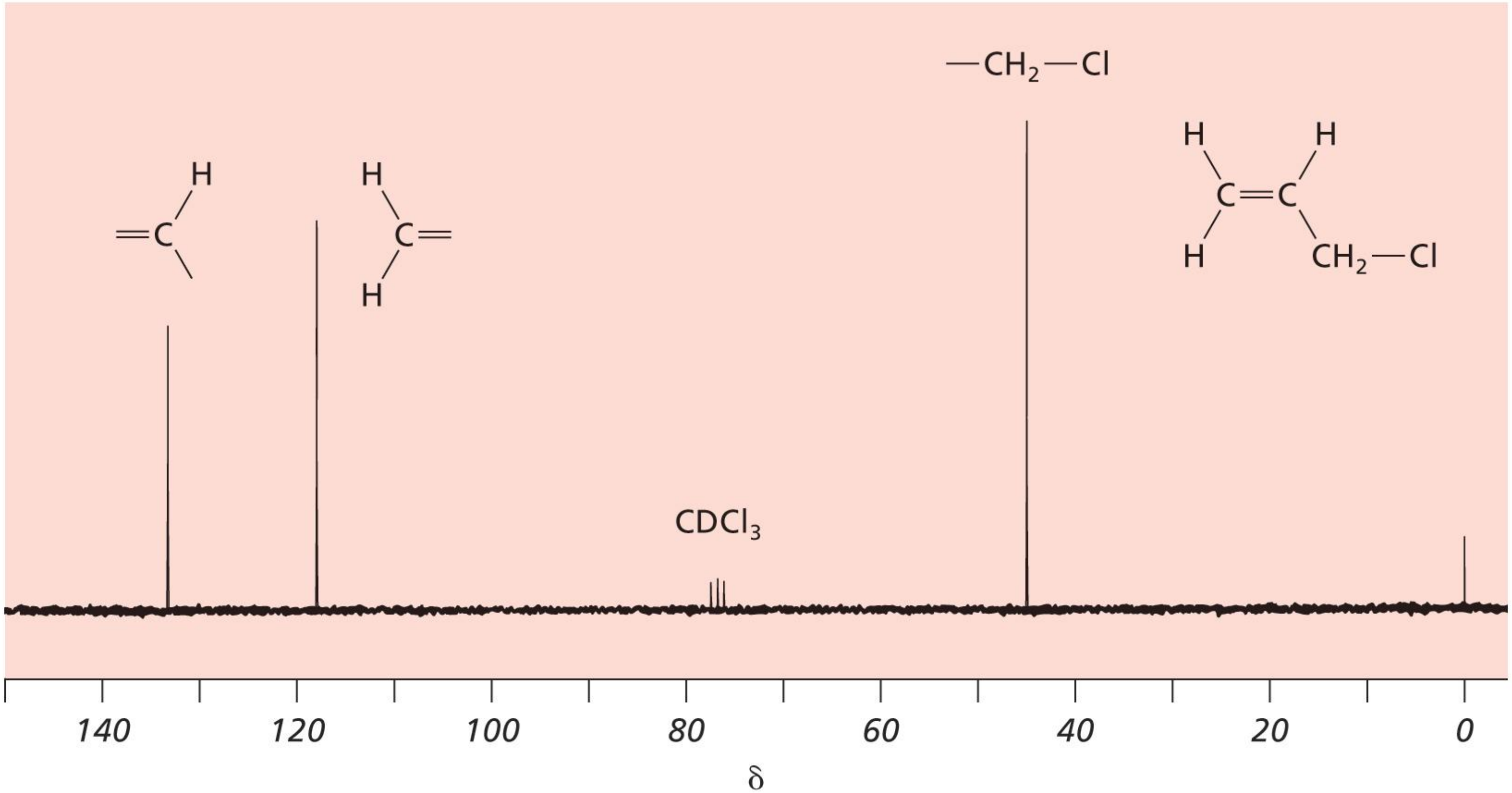
^{13}C NMR (^{1}H coupled)

$^1J_{CH}$ $^2J_{CH}$ $^3J_{CH}$

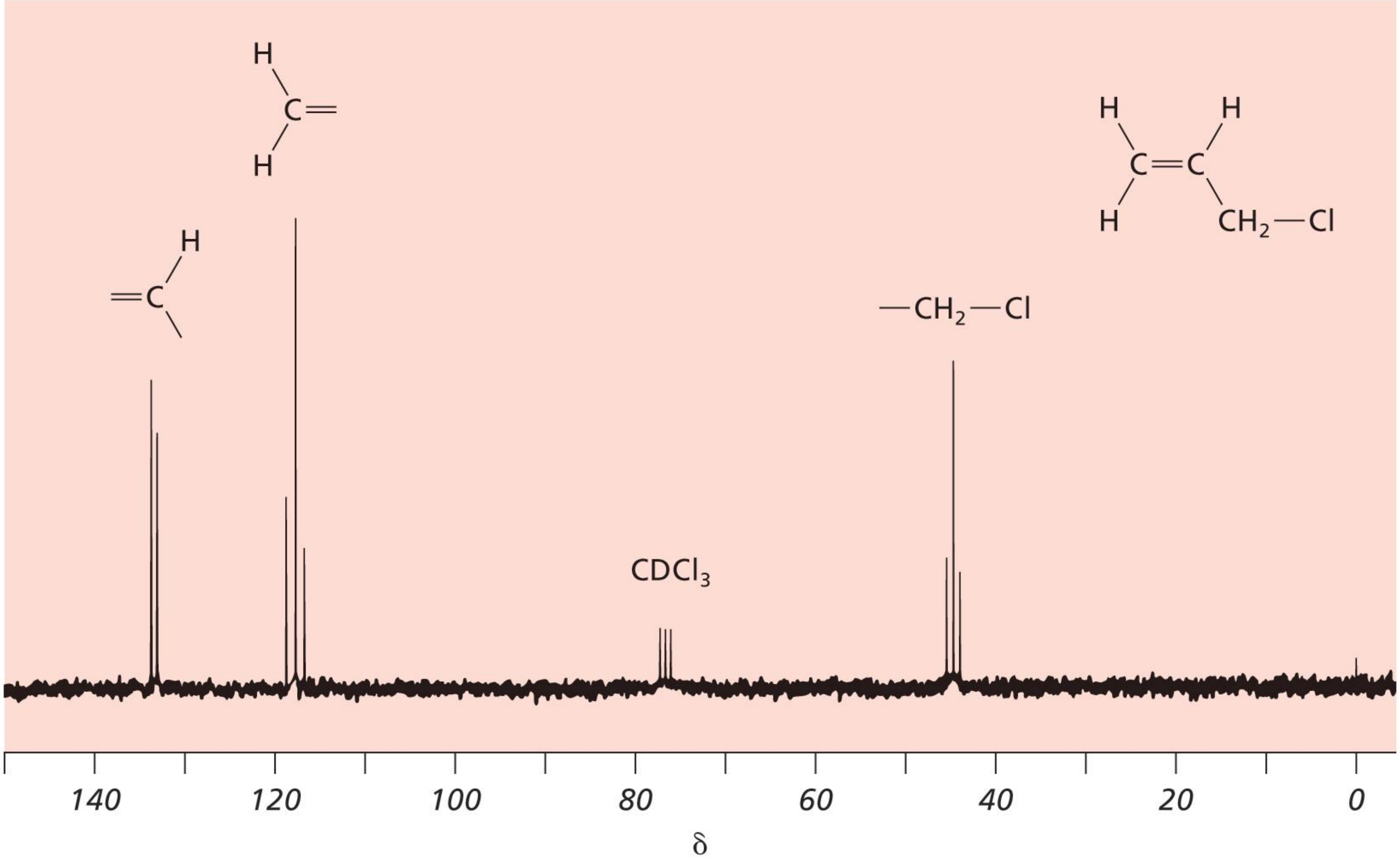
$^{13}C—H$ $^{13}C—C—H$ $^{13}C—C—C—H$



$^{13}C\{^1H\}$ NMR (^1H decoupled):

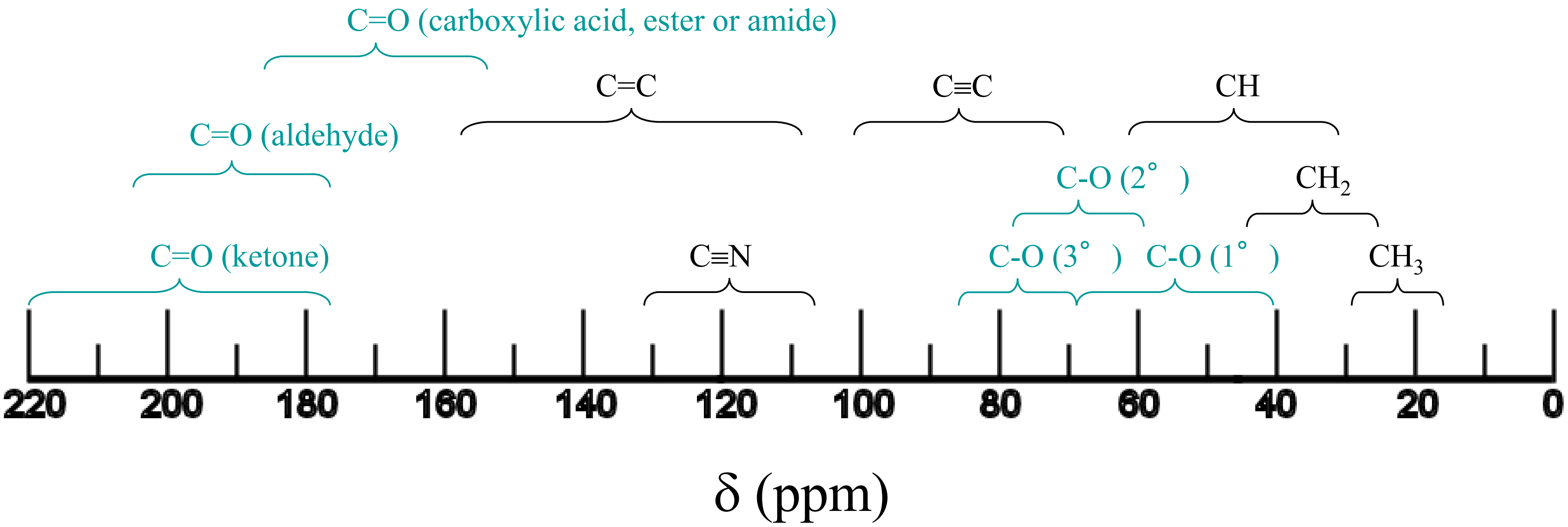


^{13}C NMR (^1H coupled – only one-bond):



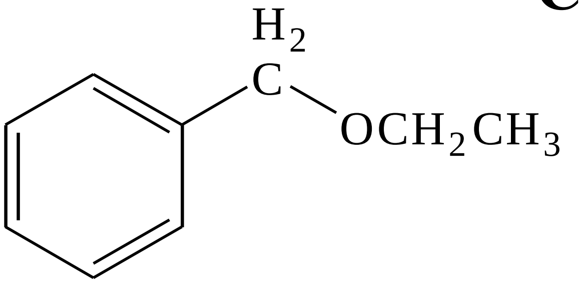
^{13}C NMR Spectroscopy

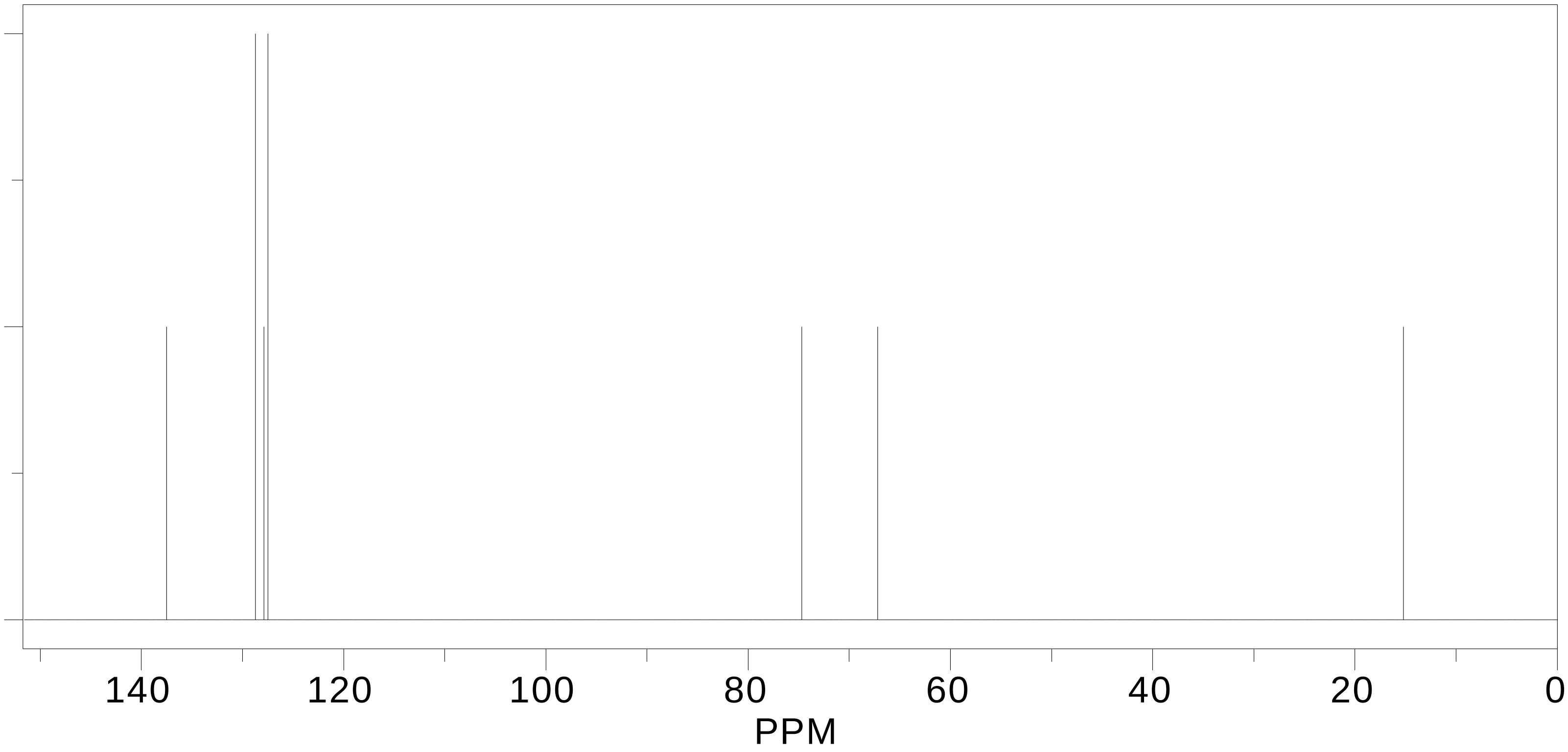
- The main utility of ^{13}C NMR is to tell us how many unique carbon atoms are in a molecule



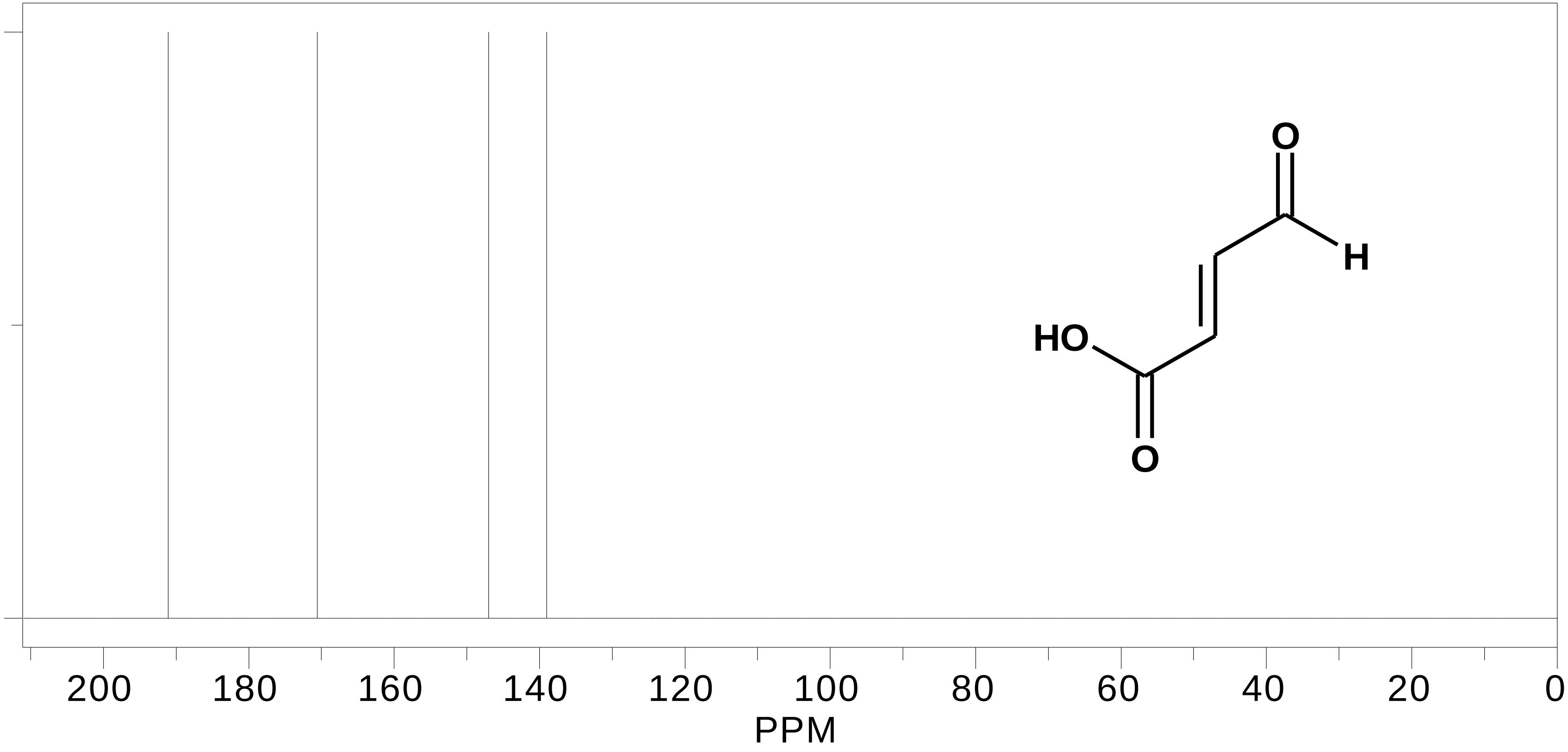
- ^{13}C NMR is particularly useful for identifying carbonyl and nitrile groups which do not show up directly in ^{1}H NMR spectra.

^{13}C NMR Spectroscopy

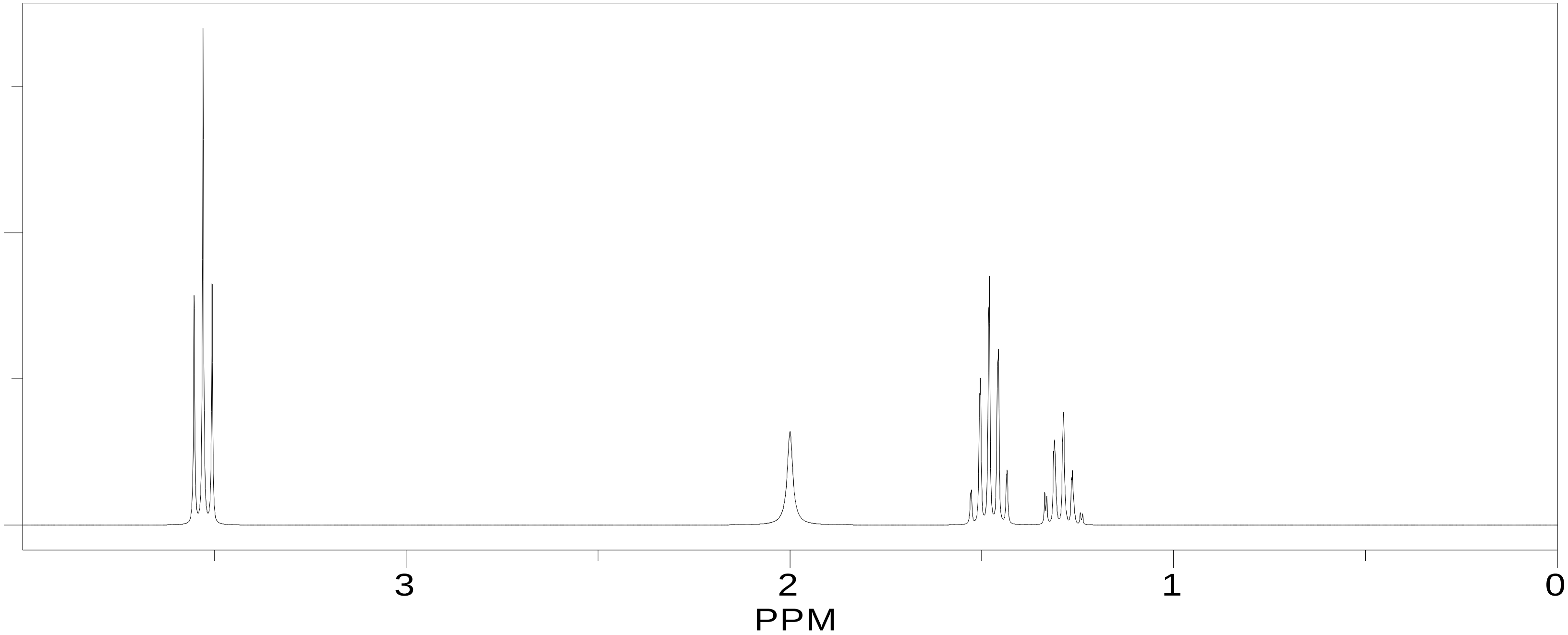


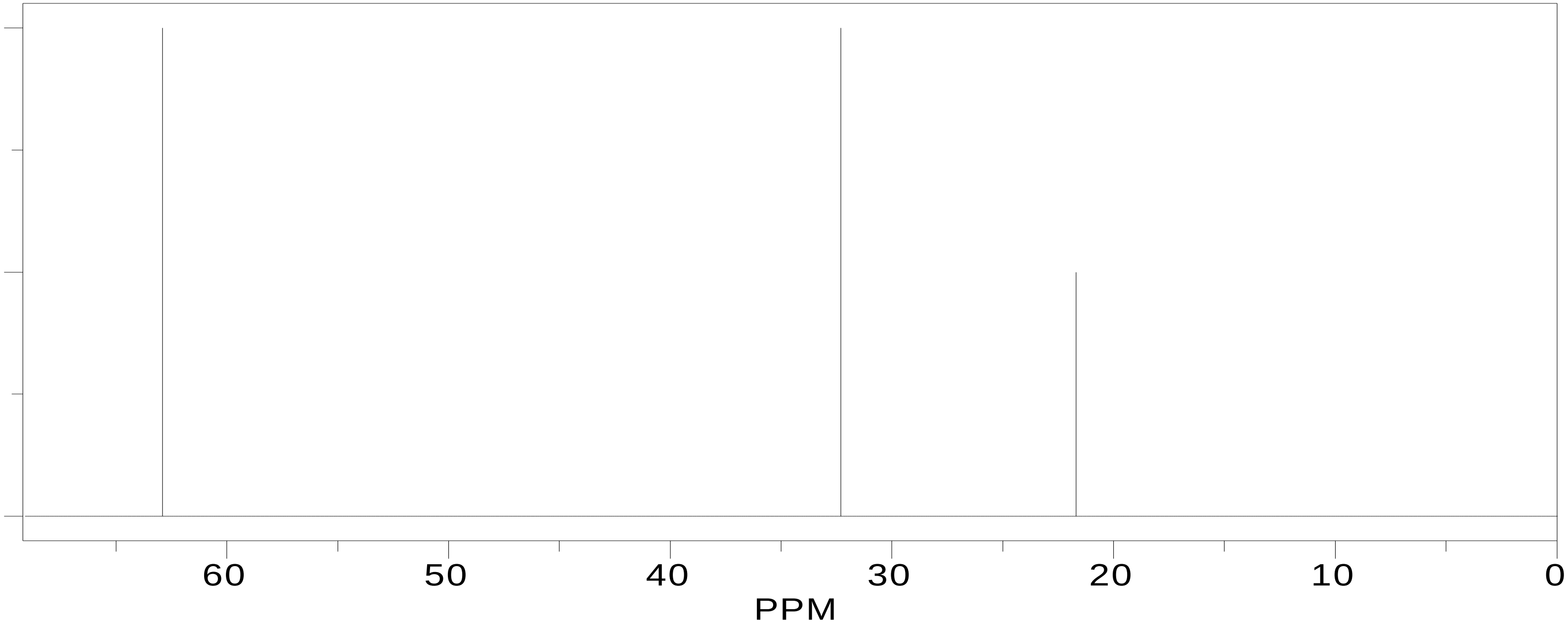


^{13}C NMR Spectroscopy

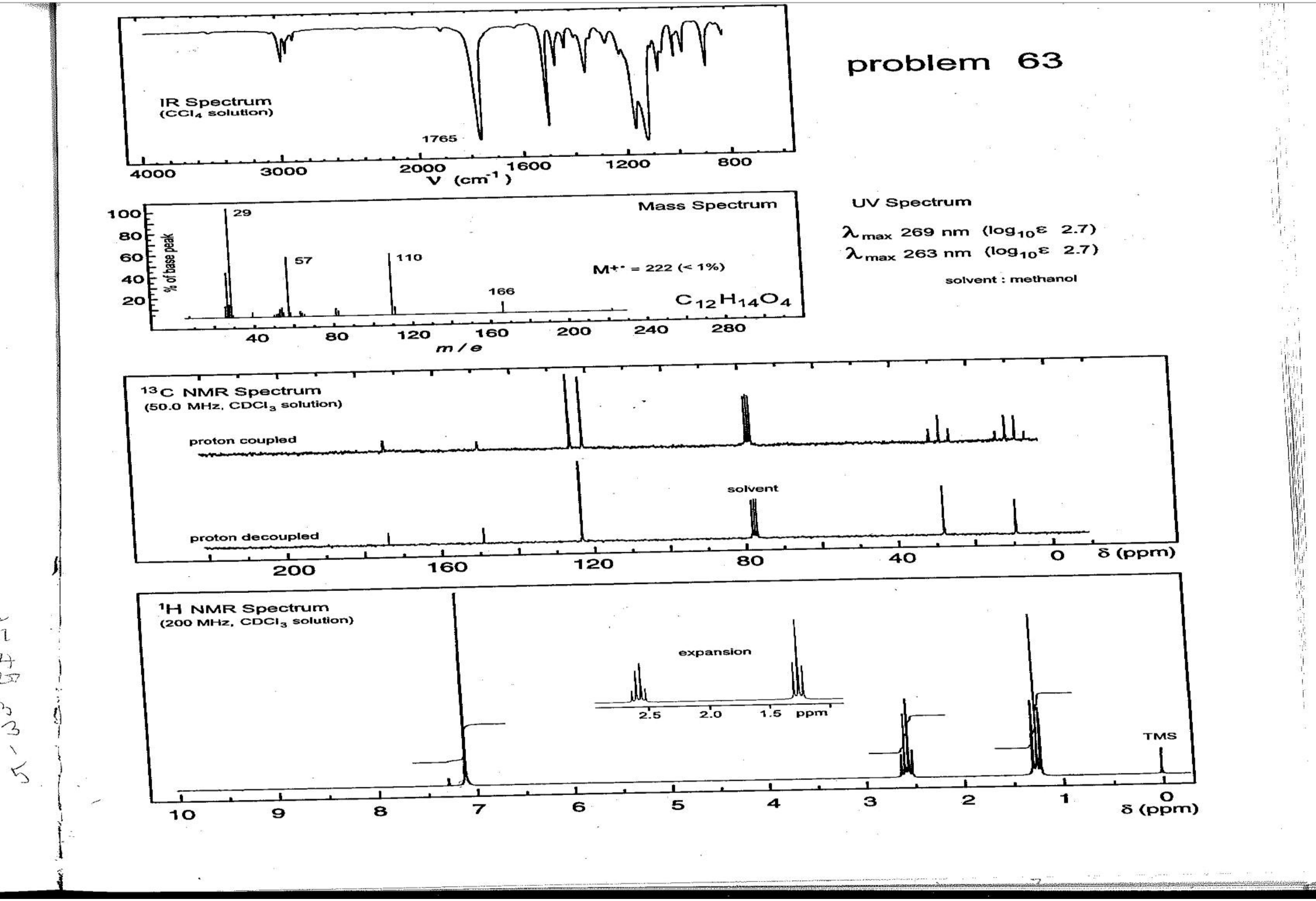


$C_5H_{12}O_2$ Int: 2:1:2:1





Practice problems with ^{1}H, ^{13}C and IR data:



problem 63

UV Spectrum

λ_{max} 269 nm ($\log_{10}\varepsilon$ 2.7)

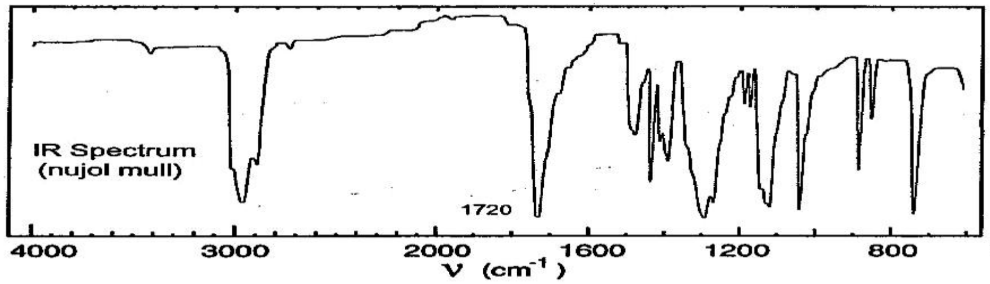
λ_{max} 263 nm ($\log_{10}\varepsilon$ 2.7)

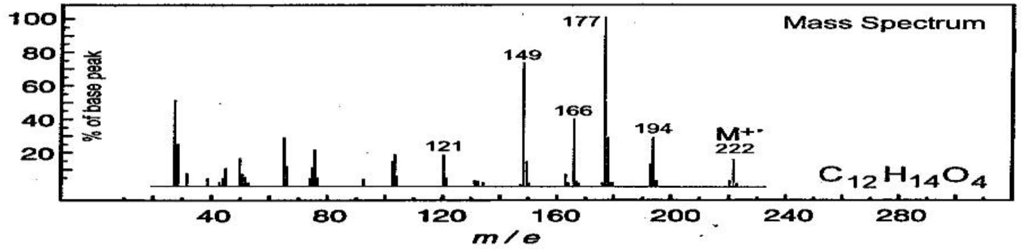
solvent : methanol

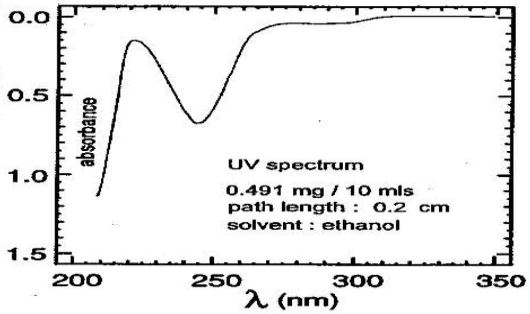
$C_{12}H_{14}O_4$

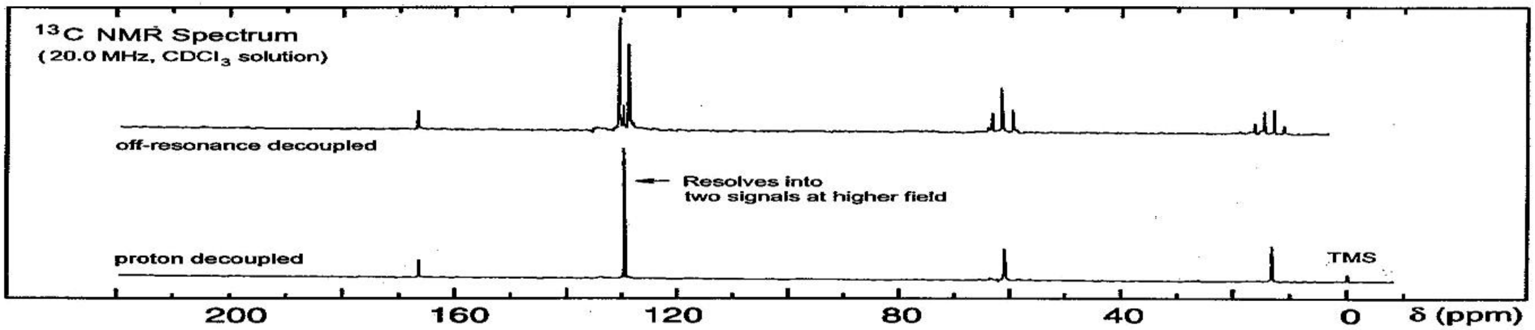
Practice problems with ^{1}H, ^{13}C and IR data:

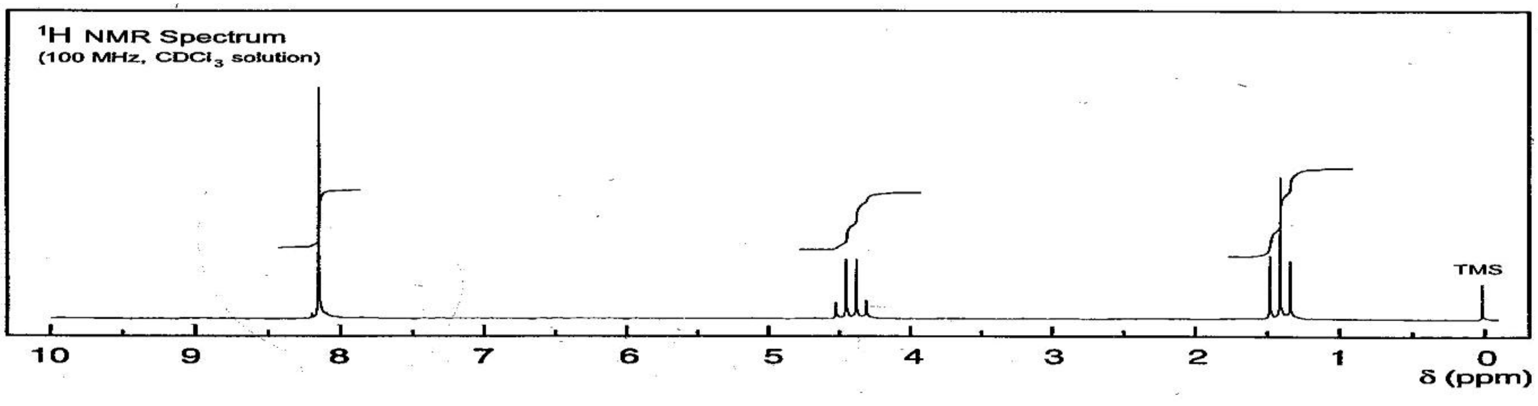
problem 64





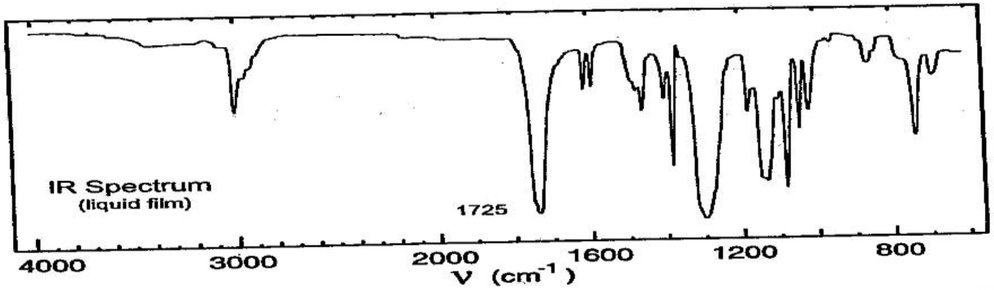


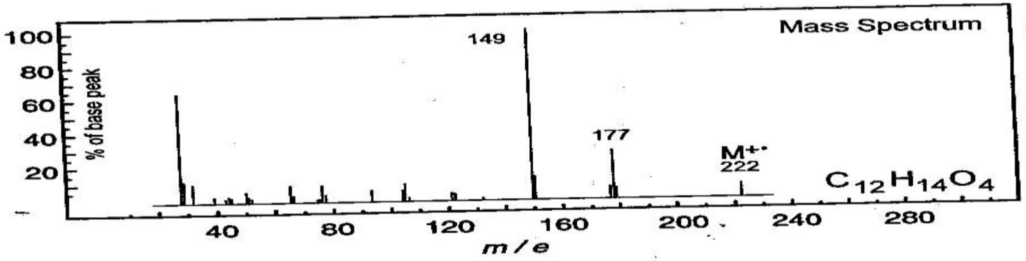


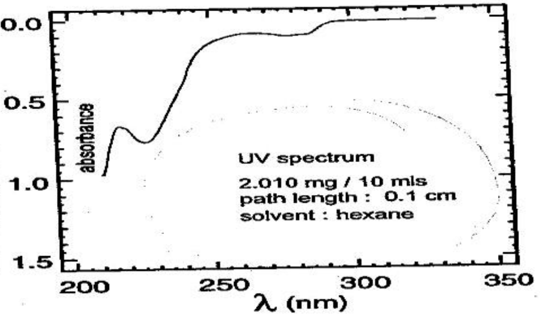


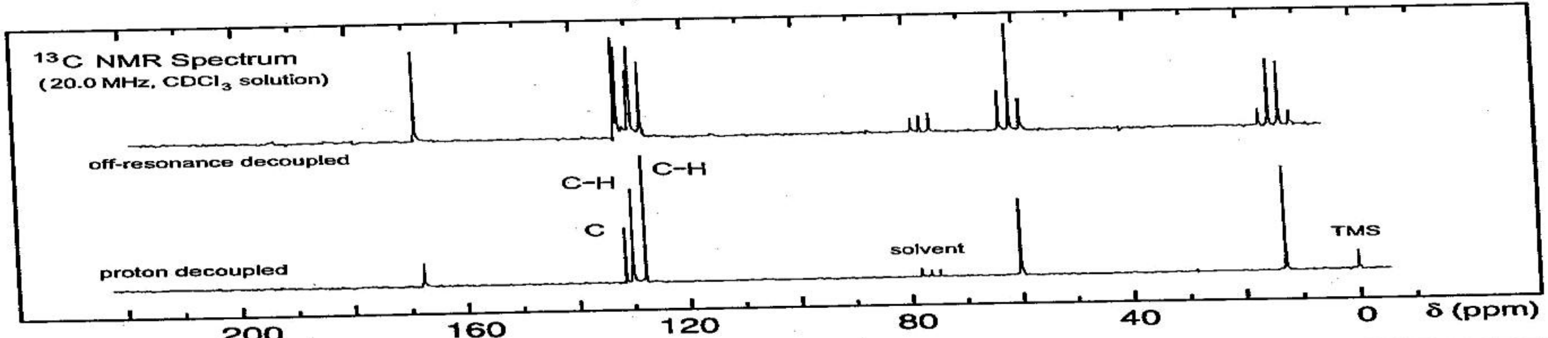
Practice problems with ^{1}H, ^{13}C and IR data:

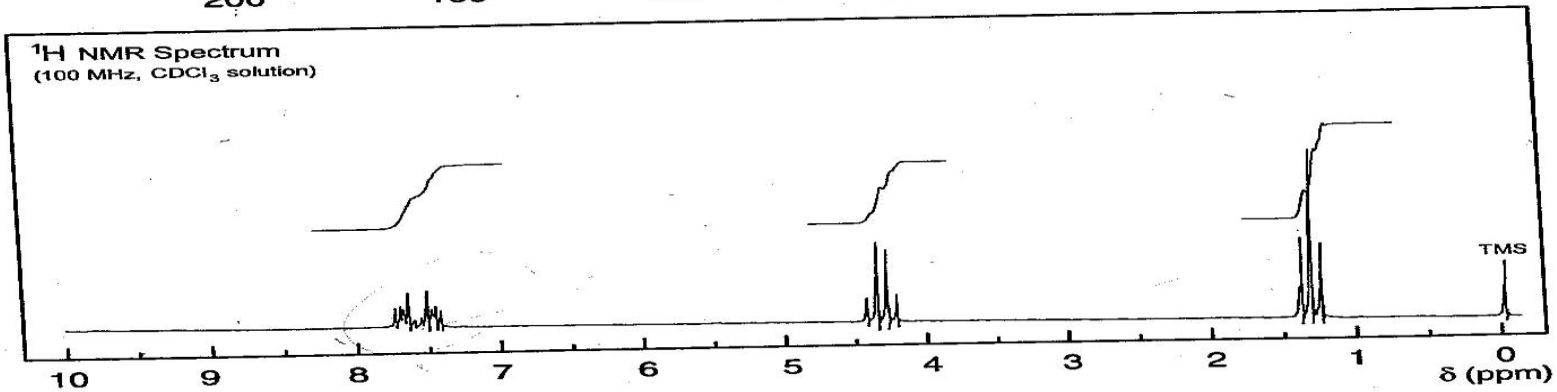
problem 65



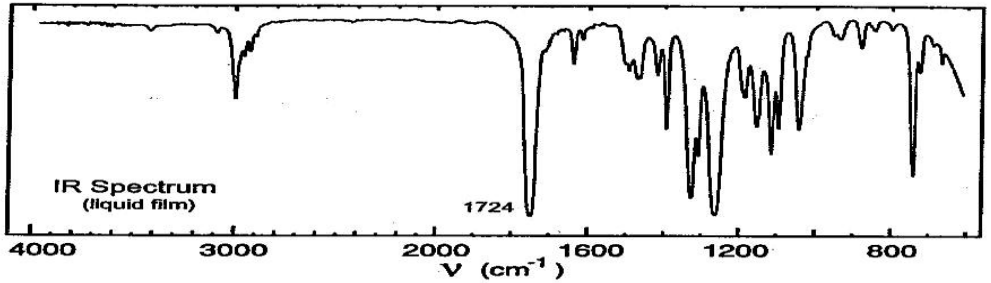








Practice problems with ^{1}H, ^{13}C and IR data:



problem 66