

The ^1H NMR spectrum provides three pieces of information:

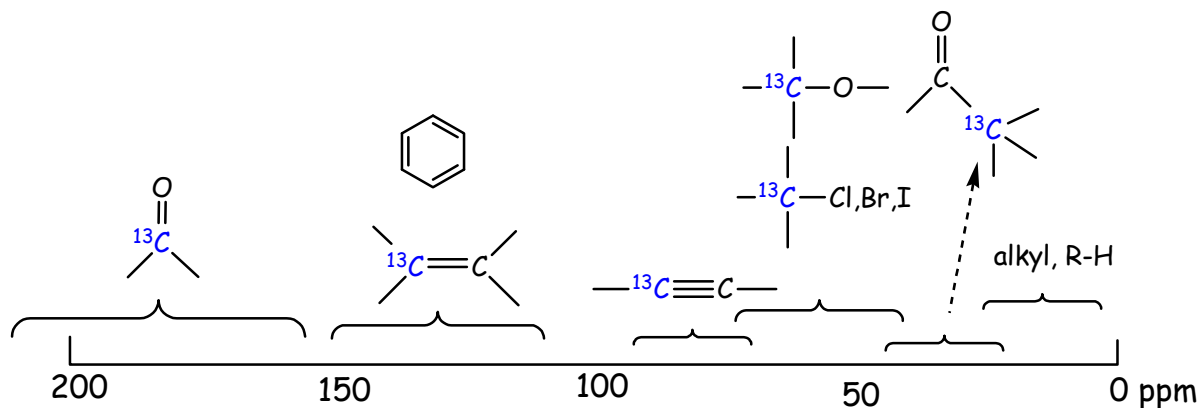
1. **chemical shift**- position of peak on the x-axis- shielding and deshielding
2. **area under the peak (integration)**- indicates the number of hydrogens in resonance at that frequency
3. **signal splitting**- multiplicity of signal- indicates the number of hydrogens on adjacent carbon atoms

Correlation Tables for ^1H chemical shifts:

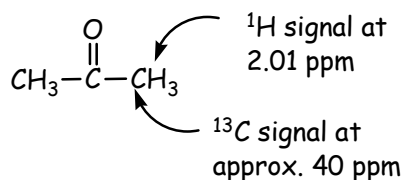
aldehydes acids	aromatic	vinyl	Z = O, N halogen	allylic	saturated
12 - 9.0	8.0 - 6.5	6.5 - 4.5	4.5 - 2.5	2.5 - 1.5	1.5 - 0

13 - 9.0	8.5 - 6.5	6.5 - 4.5	5.0 - 2.5	3.0 - 2.5	2.5 - 2.0	1.5 - 0

Correlation Tables for ^{13}C chemical shifts:



Helpful observation: The chemical shifts for ^{13}C nuclei are 15-20 times larger than the corresponding ^1H nuclei frequencies. Example: acetone. Protons next to the carbonyl observed at 2.01 ppm. The ^{13}C signal for the carbon next to the carbonyl is $2.01 \times 20 = 40$ ppm.

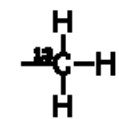


Chemical shifts for carbonyl functional groups (ppm)

ketones	220-200	amides	180-160
α,β -unsaturated ketones	210-190	acid chlorides	180-160
aldehydes	205-190	anhydrides	175-150
carboxylic acids	185-165	nitriles	120-115
esters	185-160		

Spectra which show the **spin-spin splitting**, or **coupling**, *between carbon-13 and the protons* directly attached to it are called **proton-coupled spectra** or **nondecoupled spectra**.

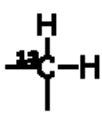
3 protons



$$n + 1 = 4$$



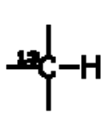
2 protons



$$n + 1 = 3$$



1 protons



$$n + 1 = 2$$



0 protons



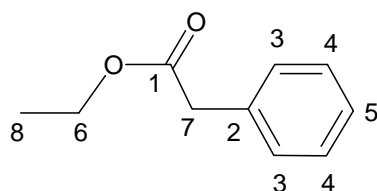
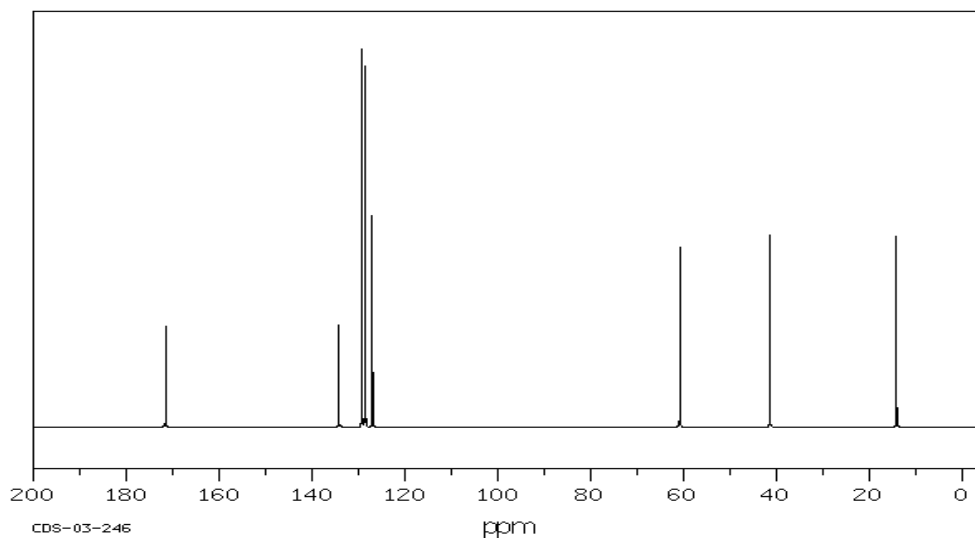
$$n + 1 = 1$$



Coupled and decoupled Spectra

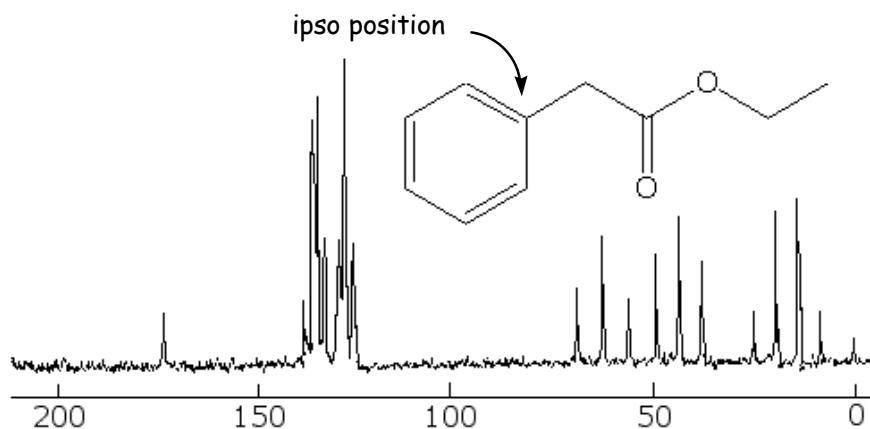
Spectra in which the protons are decoupled from the C-13 nuclei are called **proton-decoupled** spectra or simply **decoupled spectra**. Decoupled spectra show singlets for each non-equivalent carbon-13 nucleus.

Here is the **proton-decoupled spectrum** of ethyl phenyl acetate. Nice and clean!



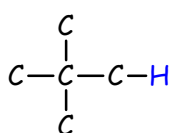
1	171.5 ppm
2	134.3
3	129.3
4	128.5
5	127.0
6	60.8
7	41.4
8	14.2

Here is the **proton-coupled spectrum** for the same compound, ethyl phenyl acetate. Notice the two triplets and a quartet for the sp^3 carbons, whereas the aromatic carbons show non-first order splitting. Also, the carbonyl carbon and the **ipso** ring carbon both have a low intensity in both spectra (no hydrogens attached to these carbons).

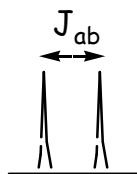
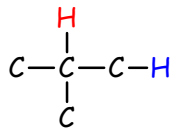


Spin-Spin Coupling

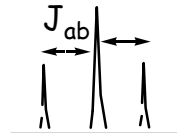
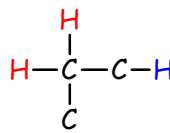
Saturated systems:



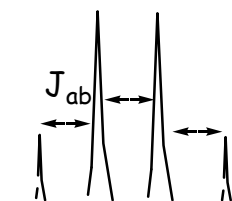
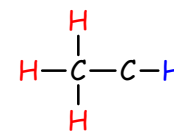
no coupled
hydrogen atoms
singlet



one coupled
hydrogen atoms
doublet

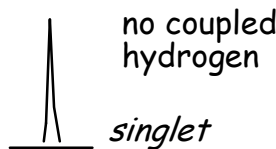
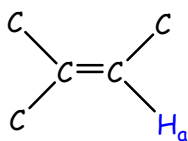


two coupled
hydrogen atoms
triplet



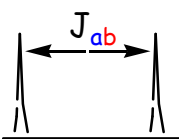
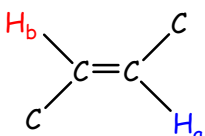
three coupled
hydrogen atoms
quartet

Vinyl systems:



no coupled
hydrogen

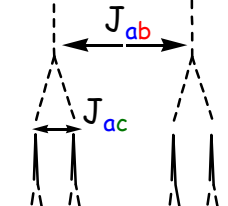
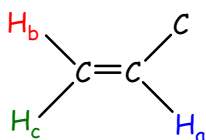
singlet



one coupled
hydrogen

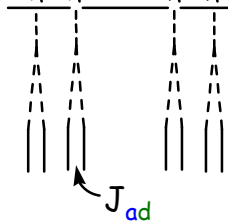
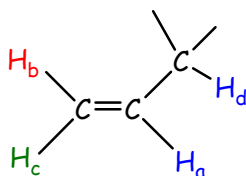
doublet

notice trans-coupling
(J_{ab}) is larger than
cis-coupling (J_{ac})



two coupled
hydrogen

doublet of doublets



three coupled
hydrogen

*doublet of
doublets of
doublets*

Common Coupling Patterns

Ethyl group: a quartet and a triplet in the ratio 2:3

The chemical shift of the CH_2 group depends on the attached substituent and ranges from:

$\delta \approx 4$ (for oxygen) to $\delta \approx 2$ (for a carbonyl).

Isopropyl group: a septet (7 peaks) and a doublet in the ratio 1:6

The chemical shift of the CH_2 group depends on the attached substituent

