

Short Summary of $^1\text{H-NMR}$ Interpretation

For fuller explanation, see: <http://www.mnstate.edu/jasperse/Chem355/H-NMR.doc.pdf>

I. Number of Signal Sets

II. Integration These must be simple whole-number ratios (2:1, 3:1, 3:2, etc..)

III. "Chemical Shifts" of the Signal Sets

9's (9.0-10.0)	<u>Aldehyde</u> sp^2 hybridized C-H's
7's (6.5-8.4)	<u>Aromatic</u> sp^2 hybridized C-H's
5's (4.8-6.8)	<u>Alkene</u> sp^2 hybridized C-H's
3's (2.8-4.5)	<u>Oxygenated</u> or <u>Halogenated</u> sp^3 hybridized C-H's (halogenated and nitrogenated alkyl C-H's will also come in this window, although no candidates for today's lab). Oxygenated sp^3 -carbons are routinely present for the following functional groups that contain oxygen single bonds: <ol style="list-style-type: none"> <u>alcohols</u>, <u>ethers</u>, or <u>esters</u>
2's (1.8-2.8)	<u>Allylic</u> sp^3 hybridized C-H's (sp^3 hybridized C-H's that has a double bond attached to the sp^3 hybridized C). Allylic signals routinely appear when one of the following double-bonded functional groups is present: <ol style="list-style-type: none"> <u>carbonyls</u>, (ketones, esters, aldehydes, acids, amides) <u>alkenes</u>, or <u>aromatics</u>
1's (0.7-2.0)	sp^3 hybridized C-H's, with <u>no attached Functional Groups</u> <ol style="list-style-type: none"> <u>Note:</u> Many molecules with non-functional alkyl portions will give a lot of signal in this area.
0-12 (anywhere!)	<u>Alcohol/Acid</u> O-H hydrogens (N-H hydrogens likewise) <ol style="list-style-type: none"> <u>alcohols</u>, <u>carboxylic acids</u>

- Recognize OH's..
- Check each of the zones. Each one gives you a yes or no answer about the presence of absence of the featured group.
- End-Check: Check that the functional groups indicated by your chemical shift information match with the structure you believe you actually have! If not, structure needs correction!
- The regions are somewhat approximate, and have some spillover.
- For multi-functional complex molecules, there are more complex ways for a C-H to come in some of the above window. For example, an sp^3 -hybridized C-H with two attached oxygens can come in the 5's, or an sp^3 -hybridized C-H that is doubly allylic can come in the 3's. In other words, the impact of functional groups is roughly additive.

IV. Splitting

- **N-1 Rule:** **N lines** \rightarrow **N-1 neighbor H's** (H's directly attached to carbons attached to the C-H group causing the signal)
 - The N-1 Rule is useful when working from spectrum to actual structure
- **N+1 Rule:** **N neighbor H's** \rightarrow **N+1 lines**
 - The N+1 Rule is useful when working from structure to actual spectrum

Note: OH hydrogens don't participate in splitting (normally)

Short Summary of C13-NMR Interpretation

For fuller explanation, see: <http://www.mnstate.edu/jasperse/Chem355/C-13%20NMR.doc.pdf>

- Count how many lines** you have. **This will tell you how many types of carbons** you have. (Symmetry equivalent carbons can at times cause the number of lines to be less than the number of carbons in your structure.)
 - Each “unique” carbon gives a separate line.
 - Symmetry duplicates give the same line.
 - If there are more carbons in your formula than there are lines in your spectrum, it means you have symmetry.
- Check diagnostic frequency windows** (“chemical shift windows”) of the lines **to provide yes-or-no answers regarding the presence or absence of key functional groups** in your molecule.

220-160	C=O carbonyl carbons, sp ² hybridized
160-100	C alkene or aromatic carbons, sp ² hybridized
100-50	C-O oxygen-bearing carbons, single bonds only, sp ³ hybridized
50-0	C alkyl carbons, no oxygens attached, sp ³ hybridized

- Check Splitting.** C13 NMR's are often acquired as “decoupled” spectra, in which each carbon signal appears as a singlet. This is the way our laboratory C13 NMR's come out. However, at the cost of extra time it is also possible to get “coupled” C13 NMR's with splitting. These splitting values are very useful, and follow the N+1/N-1 rules (the number of lines is one greater than the number of attached H's).

Quartet (q)	CH ₃
Triplet (t)	CH ₂
Doublet (d)	CH
Singlet (s)	C (no attached hydrogens).

- Signal Height/Size**
 - Carbons without any attached H's are short. This is common for carbonyls (aldehydes are the only carbonyl carbons that have hydrogens attached) and for substituted carbons in a benzene ring.
 - Symmetry duplication multiplies signal height (if you have two copies of a carbon, the line will probably be taller than normal!)
- Aromatics, Symmetry, and C-13 Signals.** Most aromatics have symmetry, and both the number of aromatic lines and the splitting of the aromatic lines can be indicative of the substitution pattern on a benzene. Mono- and para-disubstituted benzenes have symmetry.

4 lines s, d, d, d	Monosubstituted benzene. (Has symmetry).
4 lines s, s, d, d	Para-disubstituted benzene. (Has symmetry).
6 lines s, s, d, d, d, d	Ortho- or meta-disubstituted benzene. (Has no symmetry).

Summary of IR (Infrared) Interpretation

- Check for Diagnostic Signals**

3500-3200	OH or NH
1800-1640	C=O
3500-2500 + 1800-1640	CO ₂ H
- Further Information in the “Carbonyl Zone”**

<1700	Unsaturated C=O
>1700	Saturated C=O
1720-1700	Saturated ketones, aldehydes, acids
1750-1735	Saturated ester