

Summary of C13-NMR Interpretation

- 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, sp² hybridized
 160-100 C alkene or aromatic carbons, sp² hybridized
 100-50 C-O oxygen-bearing carbons, single bonds only, sp³ hybridized
 50-0 C alkyl carbons, no oxygens attached, sp³ 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) CH₃
 Triplet (t) CH₂
 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