

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.

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| 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 |

- Use DEPT and/or Coupled C13 NMR to Differentiate C, CH, CH2, and CH3 carbons.**

| <u>Type of C</u> | <u>Name</u> | <u>DEPT-135</u> | <u>Coupled C13</u> |
|------------------------------|-------------|-----------------|--------------------|
| CH ₃ | Methyl | Up | Quartert (q) |
| CH ₂ | Methylene | Down | Triplet (t) |
| CH | Methane | Up | Doublet (d) |
| C (no attached hydrogens) | Quaternary | Absent | Singlet (s) |

- 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) |

- 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!)