Summary of C13-NMR Interpretation

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

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

Type of C	Name	DEPT-135	Coupled C13
CH_3	Methyl	Up	Quartert (q)
CH_2	Methylene	Down	Triplet (t)
CH	Methane	Up	Doublet (d)
C	Quaternary	Absent	Singlet (s)
(no attached			
hydrogens)			

4. <u>Aromatics, Symmetry, and C-13 Signals</u>. 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)

5. Signal Height/Size

- a. 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.
- b. Symmetry duplication multiplies signal height (if you have two copies of a carbon, the line will probably be taller than normal!)