# I. Introduction to NMR – Carbon-13

The different kinds of information one can get from an ordinary C-13 NMR spectrum can be classified in the following 3 ways: 1) the number of different kinds of **magnetically different** nuclei in the compound, 2) the **chemical shift** of the nuclei, and 3) a rough indication of the number of absorbing nuclei via the **intensity** of the peaks. Each of these will be discussed in turn.

The **number of magnetically different nuclei** in a molecule will determine the number of peaks in the spectrum. For example, in the C1 to C4 alkyl bromides a spectrum that contains just two peaks in the carbon spectrum must be *t*-butyl bromide ((CH_3)$_3$CBr), bromoethane (CH_3CH_2Br), or 2-bromopropane (isopropyl bromide, (CH_3)$_2$HCBr). Because all three carbons in the methyl groups of *t*-butyl bromide are equivalent they will each show as a single peak in the carbon spectrum. How many different peaks will there be in the carbon spectrum of bromoethane (CH_3CH_2Br)?

Chemical Shift- the property of the absorbing nuclei that results from the electronic environment around the nucleus. Measured in parts per million with **high** chemical shift numbers being associated with nuclei **low** electron density (said to be "deshielded"). It turns out frequency is an inconvenient unit to use in NMR, but a relative scale, ppm, is very useful and easy to use. Below, "B" is field strength, and "ν" is frequency.

$$\delta = (1{,}000{,}000)\,\frac{(\text{ref B} - \text{sample B})}{\text{ref B}}\ \text{in ppm} \qquad \delta = (-1{,}000{,}000)\,\frac{(\text{ref } \nu - \text{sample } \nu)}{\text{ref } \nu}\ \text{in ppm}$$

Carbon chemical shifts:
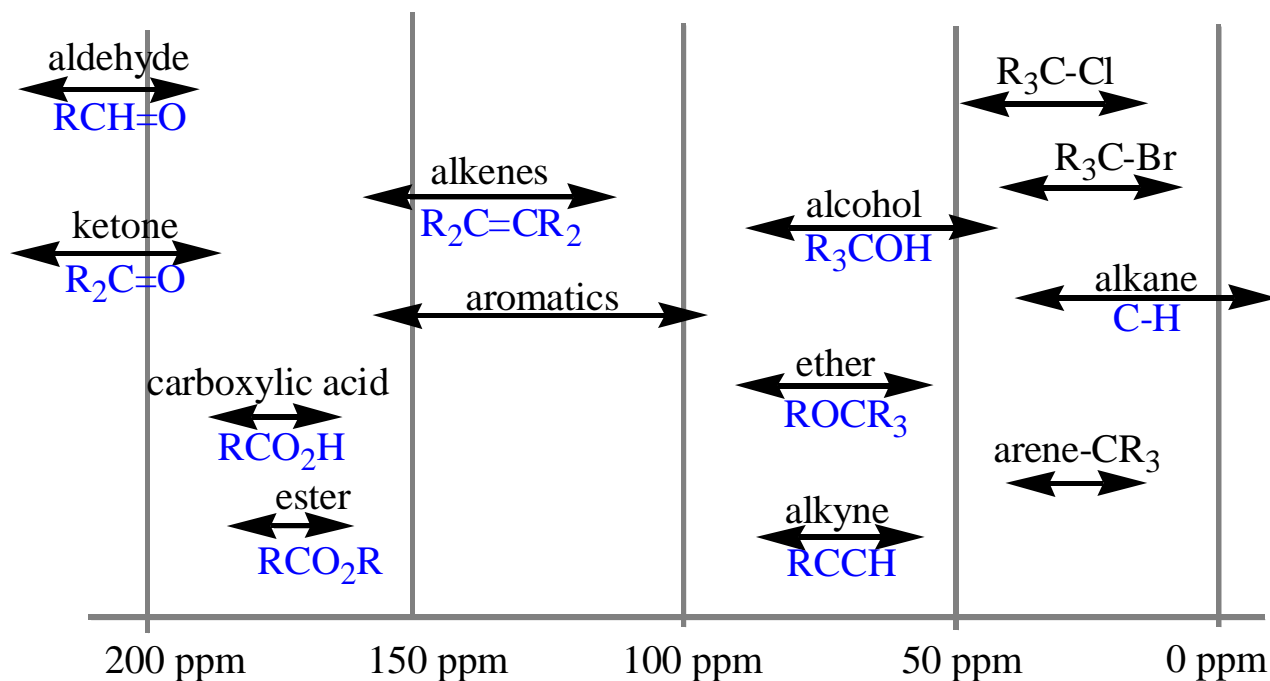
Intensity (height) of the peaks - Because of the long time it takes to quantitatively take a C-13 spectrum, carbon peaks are not normally integrated - a process that is done routinely for H-1 NMR and will be discussed next week. However, for carbons with hydrogens attached to them, the intensity of the peaks should be a rough indication of the relative number of carbons giving that peak. Each C-13 atom generates a signal, so the height of the peaks is a direct measure of the number of C-13 atoms. However, it takes a long time to collect each signal and, so, the instrument truncates data collection to speed the process. This generates error that keeps the peak heights from being a very accurate measure of the number of carbons present. Also, carbons without hydrogens attached to them (called **quaternary** carbons) will usually give much lower intensity peaks because these carbons are not enhanced by the Nuclear Overhauser Effect (NOE). There will be more on NOE in another handout.

NMR Report - Alkane Unknown

The possible compounds for known 1 and unknown 1 are:

cyclohexane	C_6H_{12}
decane	$CH_3(CH_2)_8CH_3$
dodecane	$CH_3(CH_2)_{10}CH_3$
heptane	$CH_3(CH_2)_5CH_3$
hexane	$CH_3(CH_2)_4CH_3$
methylcyclohexane	$C_6H_{11}CH_3$
octane	$CH_3(CH_2)_6CH_3$
nonane	$CH_3(CH_2)_7CH_3$
2-methylheptane	$CH_3CH(CH_3)(CH_2)_4CH_3$
2,2,4-trimethylpentane (isooctane)	
	$(CH_3)_3CCH_2CH(CH_3)_2$

Answer these questions on your spectrum if possible. No additional sheets are necessary.

What is the known or unknown number
_____ and compound name and structure?

How many different C's are present? (from the number of peaks in the C spectrum) How many C's are associated with each peak? (from the height of the peaks.

Attach the decoupled C spectrum (the normal C spectrum). Label the peaks A, B, etc. corresponding to your answer above.

Draw the structure of the known alkane and give its name and label the carbons in the structure so that they correspond to the table above.