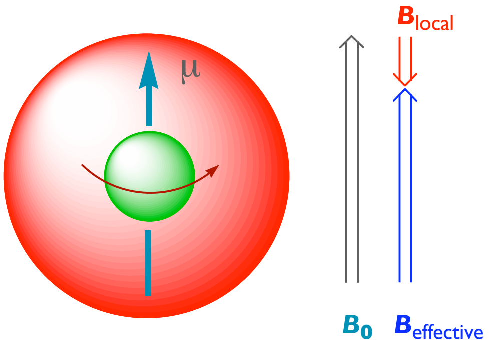
Chem 342

Lecture Summary 02
January 16, 2004

Chapter 13 - Nuclear Magnetic Resonance Spectroscopy

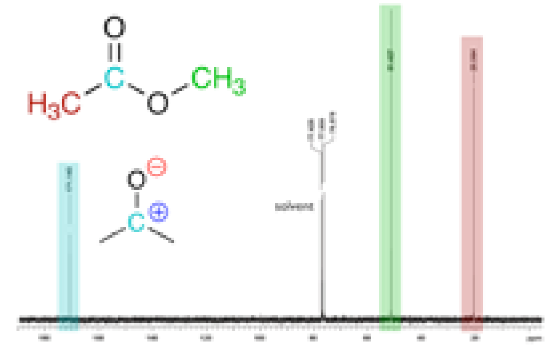
Chemical Shielding

Slight changes in this energy occur depending on the electronic environment around the nucleus. So, in ^{13}C NMR, different carbons (with different groups attached) will resonate at slightly different frequencies giving rise to separate peaks in the spectrum. The same is true for ^{1}H NMR. For example, methyl acetate carbon NMR spectron shows three different carbons - the most shielded by electrons occurs further to the right and the least shielded (most deshielded) lies on the left end of the spctrum.



$B_{effective} = B_0 - B_{local}$

Actual magnetic field felt by the nucleus

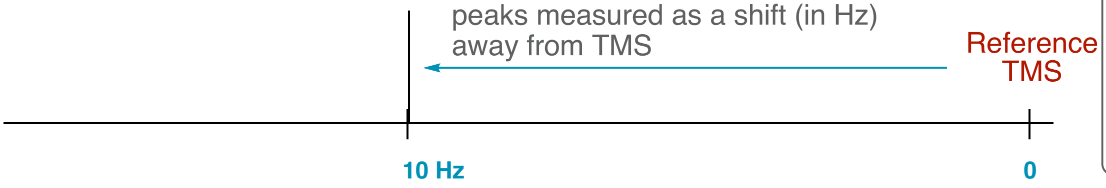


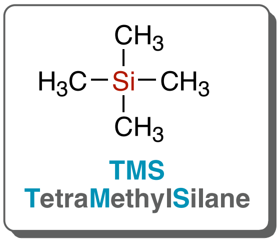
Chemical Shift and the NMR Scale

On the NMR, the peaks associated with different nuclei are measured relative to a standard molecule. For ^{1}H and ^{13}C NMR, this standard is Tetramethylsilane (TMS). This standard is set as 0 on the spectrum. Peaks from our analyte are measured as a Chemical Shift (in Hz) away from the standard.

NMR Spectrum

Low Field	**High Field**
Little electron shielding	**More electron shielding**
(more electron withdrawing groups)	(less electron withdrawing groups)





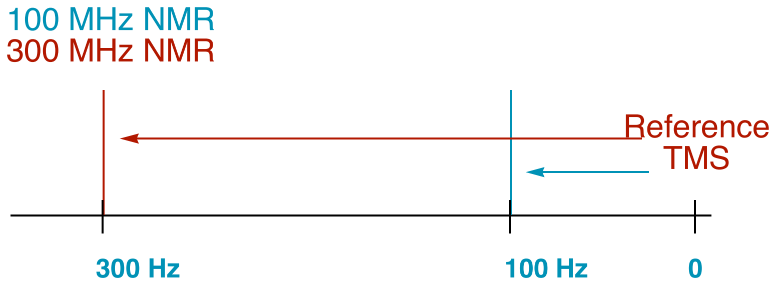
TMS
TetraMethylSilane

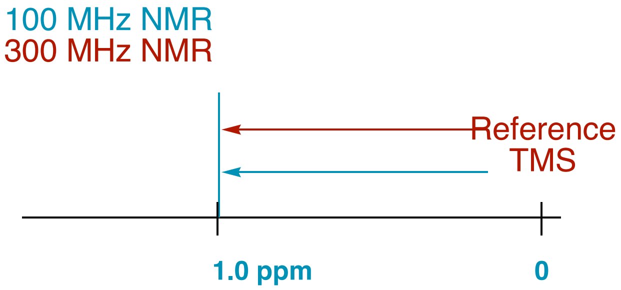
Different spectrometers would show the same peak at different chemical shifts. Thus, the scale is normalized to remove the instrument dependence. The scale (ppm - part per million) is one millionth of the particular instrument frequency.

$$\delta = \text{ppm} = \frac{\textbf{Chemical Shift from TMS (Hz)}}{\textbf{Spectrometer Frequency (MHz)}}$$

$$\frac{100\ \text{Hz}}{100\ \text{MHz}} = 1.0\ \text{ppm}$$

$$\frac{300\ \text{Hz}}{300\ \text{MHz}} = 1.0\ \text{ppm}$$



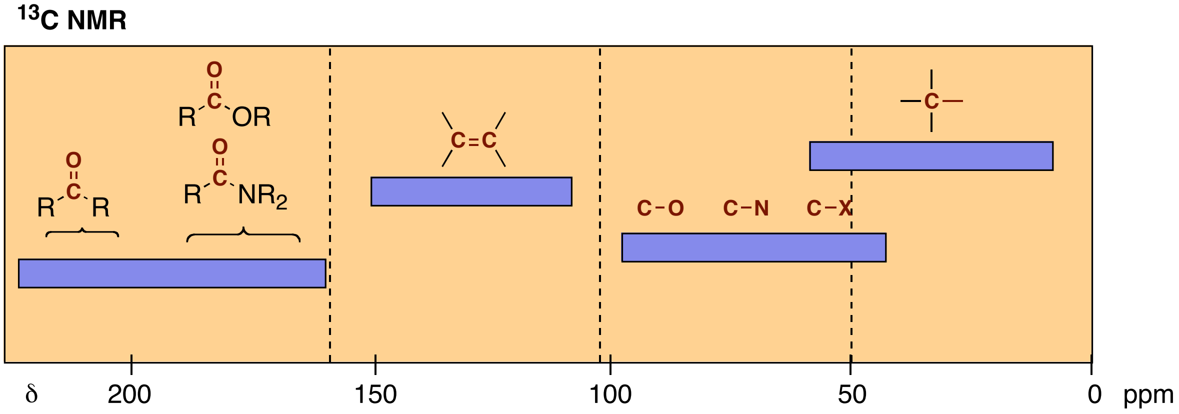


^{13}C NMR Spectroscopy

Carbon 13 makes up 1.1% of all naturally occurring carbon isotopes.

^{13}C NMR is most important for providing the number of *different* carbons, and some information about functional groups.

The ^{13}C NMR scale spans the range of about 0-200. Most shielded (alkanes) show up on the right. As electronegative subsituents are added, that shifts the resonances to the right. The alkene regions is very distinct as is the carbonyl region (most deshielded).



Carbons which are related by symmetry (mirror plane) are chemically equivalent and show up as one peak.