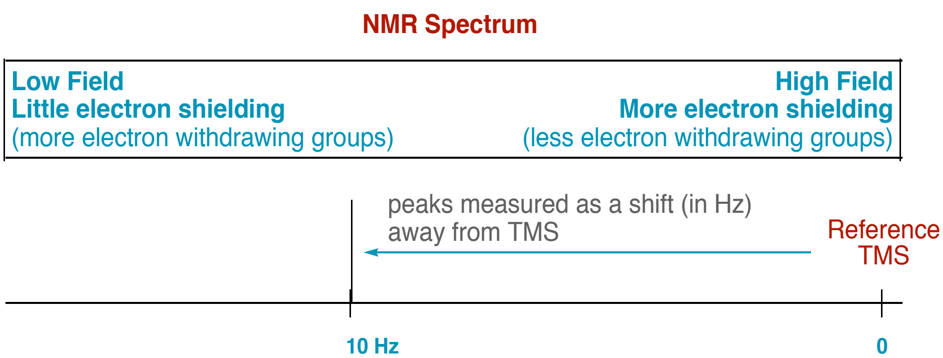
Chem 342 • Organic Chemistry II

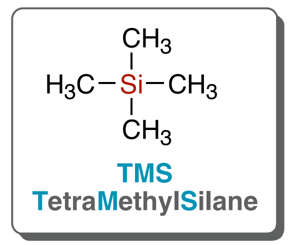
Lecture Summary 02 - 16 Jan 2009

Chapter 13 - Nuclear Magnetic Resonance Spectroscopy

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.



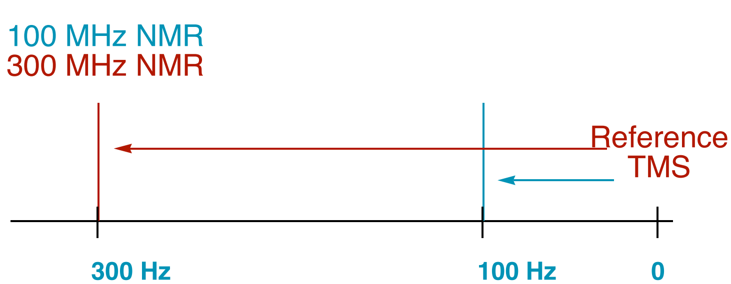


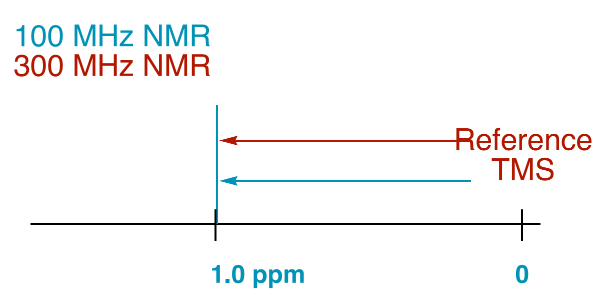
Different spectrometers would show the same peak at different chemical shifts. Thus, the scale is normalized to remove the instrument dependence. The scale (ppm - part per million) is one millionth of the particular instrument frequency.

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

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

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



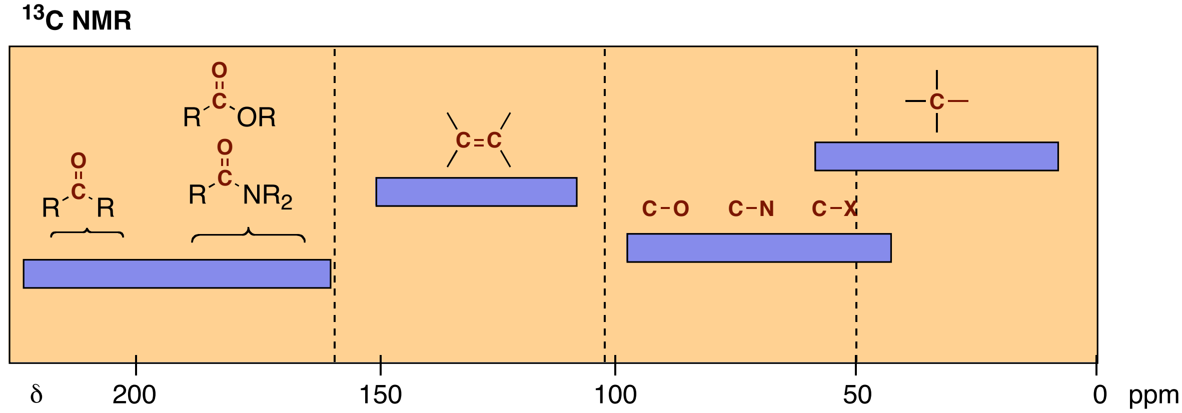


^{13}C NMR Spectroscopy

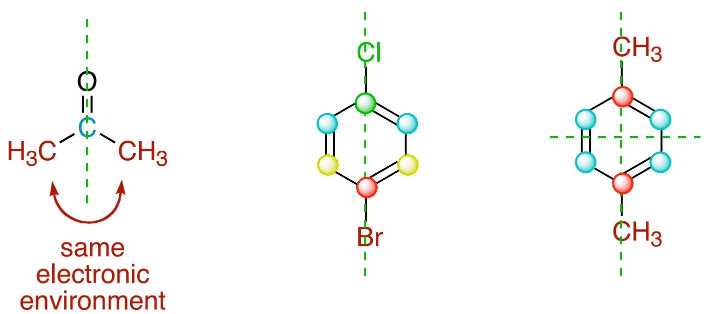
Carbon 13 makes up 1.1% of all naturally occurring carbon isotopes.

^{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.



The intensity of peaks in the carbon 13 NMR has a loose correlation with the number of H's attached to that carbon. In particular, carbons with no hydrogens on them are usually small peaks.

A DEPT spectra (Distortionless Enhancement by Polarization Transfer) can tell you how many different H's are attached to each carbon. In a DEPT experiment, three spectra are displayed. One shows all the different carbons in the molecule, one shows only the carbons with ONE hydrogen attached. The third shows all carbons with an odd number of H's attached as a positive peak (CH and CH_3) and carbons with an even number (CH_2) as a negative peak.

Recognize the chemical shifts as it relates to functional group changes (see NMR handout).

Simple symmetry information (number of different carbons) can tell you a lot.