Chem 342 Organic Chem II

Lecture Summary 05
18 Jan 2002

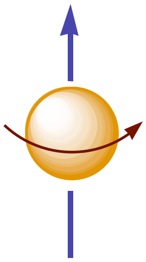
These notes can be obtained at: http://www.ndsu.nodak.edu/instruct/grcook/chem342/notes.shtml

Chapter 13: Nuclear Magnetic Resonance Spectroscopy

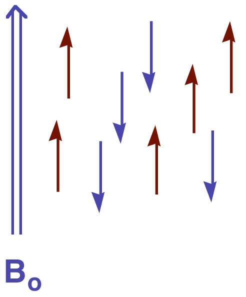
NMR Spectroscopy

Provides detailed information about the structure of molecules

The NMR phenomenon occurs due to the spins of nuclei. A charged particle (like a proton) has a spin. This generates a magnetic field with a vector component. If a molecule is placed in an applied magnetic field (B_o), the nuclear spins can align with the field or against the field.

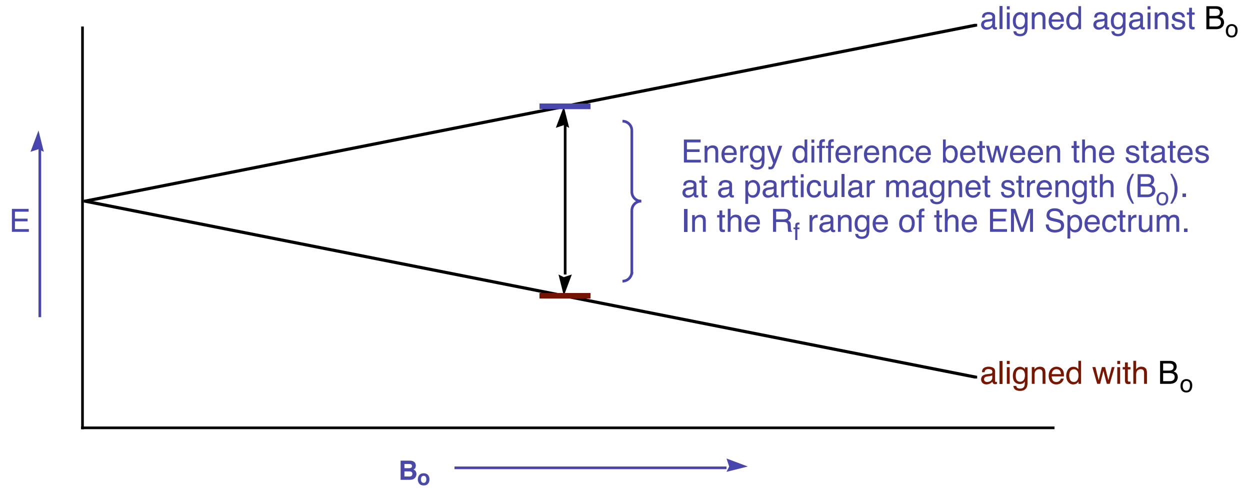


A spinning nucleus (which is charged) generates a magnetic field

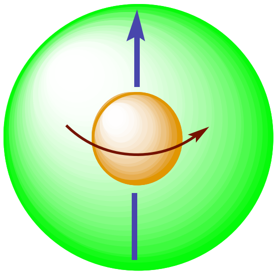


When a molecule is placed in an external magenetic field, the nuclear spins will align with or against this field

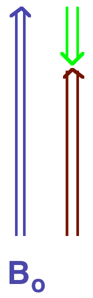
Those nuclei that are aligned with the external field are lower in energy than those opposed to the applied magnetic field. This energy is in the range of radio frequencies. Thus, when radio waves are passed through the sample, the frequency corresponding to this energy difference will be absorbed and cause the spins to flip - this is termed resonance.



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.



nuclei are surrounded by electron clouds which shield the nucleus from the magnetic field

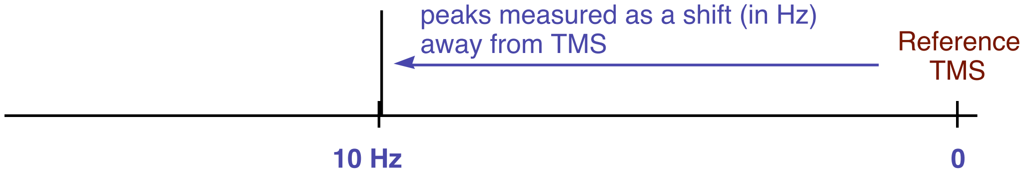


The magnetic field that a particular nucleus feels is less than B_o because of the eletron shielding. This makes every H or C in the molecule that have different electron densities around them resonate at different frequencies.

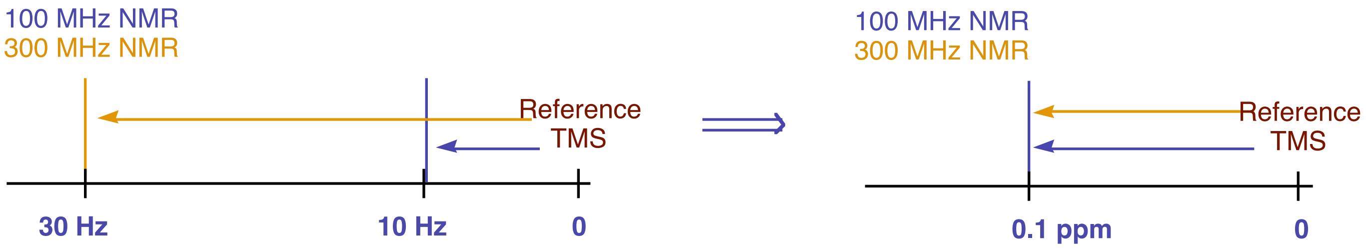
On the NMR, the peaks associated with different nuclei are measured relative to a standard molecule. For ^{1}H and ^{13}C NMR, this standard is Tetramethylsilane. This standard is set as 0 on the spectrum. Peaks from our analyte are measured as a Chemical Shift (in Hz) away from the standard.

NMR Spectrum

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



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.



$$\delta = \text{ppm} = \frac{\text{Chemical Shift from TMS (Hz)}}{\text{Spectrometer Frequency (MHz)}} \qquad \frac{10\ \text{Hz}}{100\ \text{MHz}} = 0.1\ \text{ppm} \qquad \frac{30\ \text{Hz}}{300\ \text{MHz}} = 0.1\ \text{ppm}$$