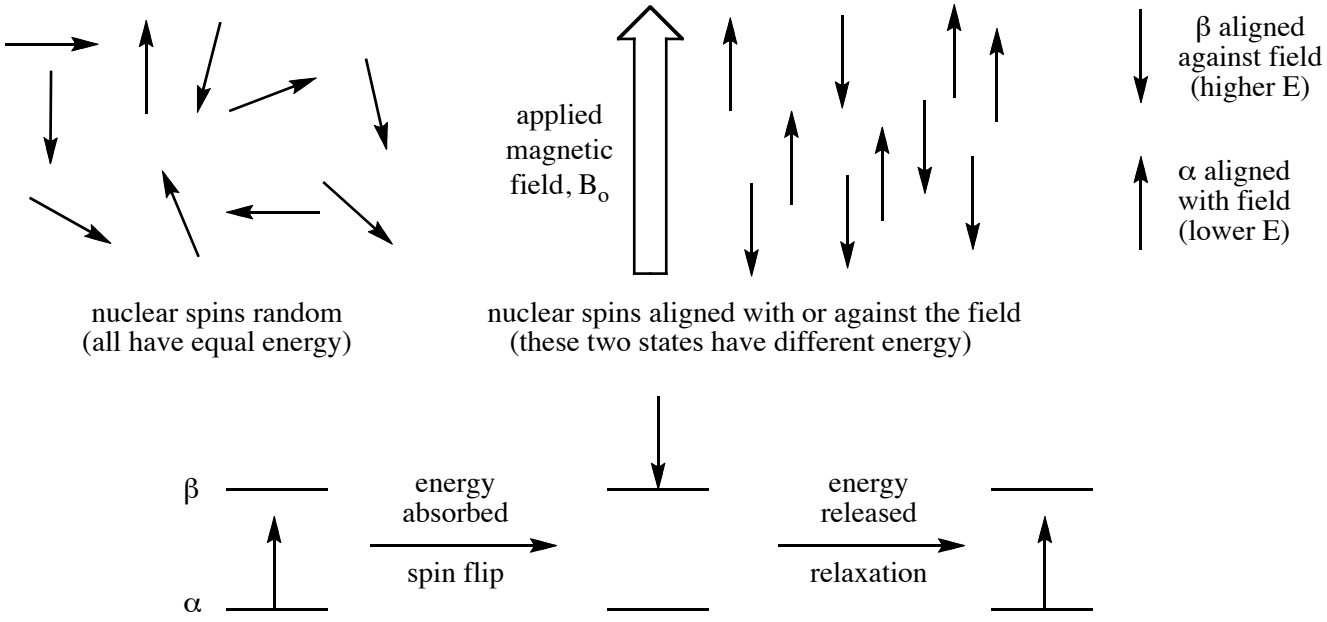
Introduction to Nuclear Magnetic Resonance (NMR) Spectroscopy

Dr. Laurie S. Starkey, Cal Poly Pomona

Like all spectroscopic methods, NMR involves the use of energy to excite a sample. By observing this interaction, we can learn something about the structure of the sample. In IR spectroscopy, absorption of IR light leads to bond vibrations (stretching and bending). In NMR, radio frequency waves are used (60,000,000 Hz or 60 MHz, also 200, 360, 500, etc.) and the resulting motion is a change in the spin of the nucleus. The nuclei which can be observed include ^{1}H (proton), ^{13}C (C-13), ^{15}N, ^{19}F, ^{31}P. These all have magnetic moments (like tiny magnets) and will interact with an applied magnetic field. Each of these nuclei has a spin quantum number I=1/2 and has **two** spin states of equal energy. When a magnetic field is applied, these spin states will align **with** or **against** the field. Those aligned with the field (**α**) are lower in energy than those aligned against the field (**β**); the difference in energy between α and β is proportional to the strength of the magnet used. Application of radio waves (energy) at just the right frequency will cause certain nuclei to absorb energy and "flip" from the α to the β spin state. As the excited nucleus relaxes back to the ground state, a signal is recorded and an NMR spectrum can be obtained. The frequency of this energy transition depends on the electronic environment of the nucleus.



Information obtained from a ^{1}H NMR spectrum:

1) **# of signals** indicates the number of different types of hydrogens (consider chemical equivalence).

2) **Integration** or peak area indicates how many hydrogens are in each signal. It is given as a ratio.

3) **Chemical shifts** are given as δ (delta) values, in ppm. The chemical shift indicates the electronic environment of the hydrogens (electron-rich/shielded or electron-poor/deshielded).

4) **Splitting patterns** indicate the # of *neighboring* hydrogens. The magnitude of the coupling constants (given as *J* values) depend on the spatial relationship (dihedral angle) of the two hydrogens.