Physical Chemistry Notes - NMR, Magnetic Splitting, Energy Levels, Resonant Frequency and Larmor Frequency.

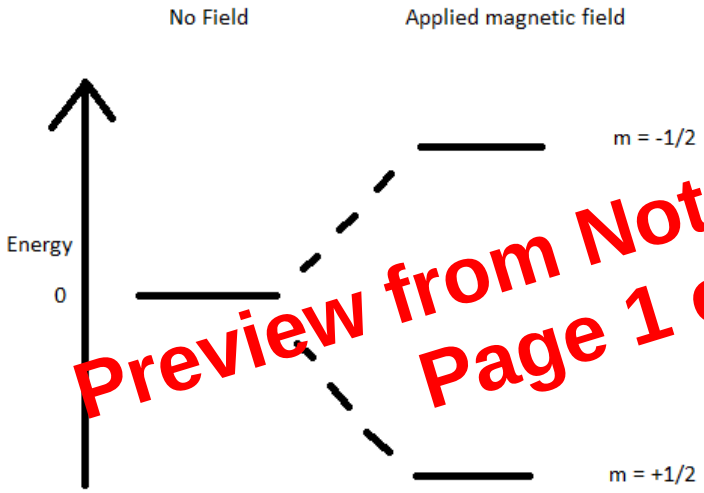
Nuclear Magnetic Resonance

- Protons and neutrons possess a spin. In many atoms e.g. ^{12}C these are paired and opposing and nucleus has no overall spin. However;
  - If number of neutrons n_N and number of protons n_p are both even then nucleus has no spin
  - If $n_N + n_p$ results in an odd total, then nucleus has half integer spin (1/2, 3/2, 5/2...)
  - If n_N and n_p are both odd, nucleus has integer spin (1, 2, 3...)

Magnetic Splitting

- A necleus of spin I has (2I + 1) possible orientations, so nucleus of I = 1/2 has 2 possible orientations - "spin up" and "spin down". In the absence of a magnetic field, these have equal energy.

In presence of a magnetic field, energy levels split, with spin +1/2 state at lower energy (aligned with the field) and spin -1/2 state at higher energy (opposed to field). According to Boltzman distribution, lower state will have a greater population.



The energy levels for a nucleus with spin quantum number 1/2

Energy levels

- Difference in energy levels produced by magnetic field is: $\Delta E = \frac{\gamma h B}{2\pi}$
  - B is the magnetic field at nucleus measured is teslas (T)
  - γ is magnetogyric ratio of the nucleus
- If B increases and γ is large energy gap is larger
  - h = plancks constant = 6.626×10^{-34} m^2 kg/s
  - For proton; γ = $2.6752 \times 10^{8} T^{-1} S^{-1}$, so for 1 T field ΔE = 2.82×10^{-26} J (corresponding to a frequency of 43 MHz). The difference in population between the 2 levels will be very small.