# Nuclear Magnetic Resonance (NMR) Spectroscopy – An Introduction

Certain nuclei are considered to spin. Spinning of a charged particle generates a *magnetic moment* along its axis of spin. These nuclei act like little bar magnets.

I (spin) $= 0$: ^{12}C, ^{16}O
$I = \frac{1}{2}$: ^{1}H, ^{19}F, ^{13}C

If a nucleus with $I = \frac{1}{2}$ (e.g. a proton) is placed in an external magnetic field, according to quantum mechanics two orientations of the magnetic moment are possible:
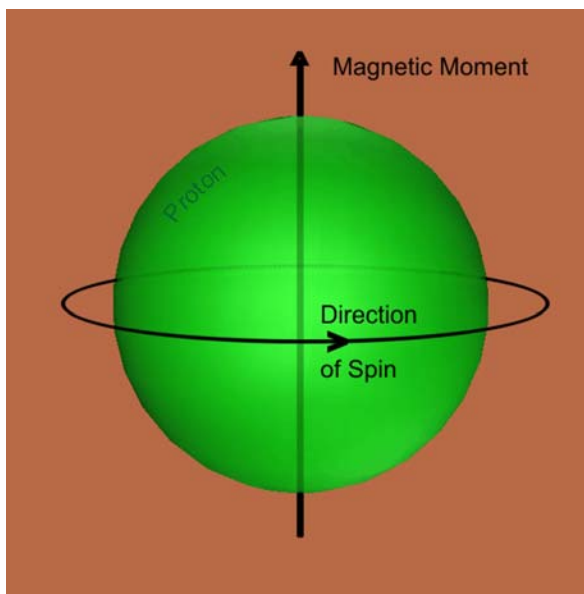
⬆ and ⬇

with external field ⬆.

The first state, ⬆, is slightly more stable than the second, ⬇; hence there are slightly more nuclei in this state.

If protons are irradiated with electromagnetic radiation of the proper wavelength, protons in one state will "flip" over to the other state.

The probability of "flipping" is independent of state, but since there are more protons in the lower energy state, there will be a net absorption of energy – this absorption of energy gives rise to the NMR signal.

The required frequency (cps or Hz) of this radiation lies in the radio frequency portion of the electromagnetic spectrum and is given by the formula: $\nu = \gamma H_n/2\pi$,

where, H_n = strength of the magnetic field at the nucleus, in gauss, and γ = the gyromagnetic ratio = 26,750 for the proton.

ν = 60MHz when H_n = 14,092 G <classic NMR instruments
ν = 300MHz when H_n = 70,460 G < current OSC NMR

To obtain a spectrum –

Place proton in 70,460 gauss field and sweep frequency of electromagnetic radiation through 300 MHz – at 300 MHz a signal will result.

Or, hold radio frequency constant at 300MHz and sweep the magnetic field through 70,460 gauss.

Absorption ↑

Magnetic field ⟶ Or radio frequency
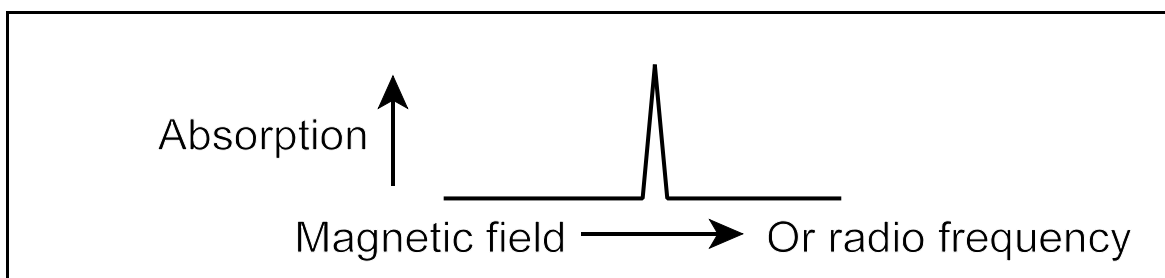
In the case of a molecule in an external magnetic field, electrons circulate and generate (small) *induced magnetic fields*. Electrons around a proton generate an induced field which opposes the applied field (from the spectrometer magnet) at the proton – we say the proton is *shielded*.

If H_o is the applied field and H_i is the induced field at the proton caused by the electrons, then the actual field at the proton, $H_n = H_o - H_i$.

Compared to a naked proton, a shielded proton requires a higher H_o to provide the H_n at which absorption occurs. Different protons in a molecule will have different amounts of shielding and will absorb at different values of H_o, giving rise to the proton NMR spectrum.

This story is much the same for any nucleus that has a spin of ½, ^{13}C, for example.