

- Relative sensitivity

- Compare ^1H , ^{31}P

$$\gamma(^1\text{H}) = 267.522 \times 10^6 \text{ s}^{-1} \cdot \text{T}^{-1}$$

$$\gamma(^{31}\text{P}) = 108.394 \times 10^6 \text{ s}^{-1} \cdot \text{T}^{-1}$$

$$\frac{\gamma(^1\text{H})}{\gamma(^{31}\text{P})} \approx 2.5$$

- Compare ^1H , ^{13}C

$$\gamma(^1\text{H}) = 267.522 \times 10^6 \text{ s}^{-1} \cdot \text{T}^{-1}$$

$$\gamma(^{13}\text{C}) = 67.283 \times 10^6 \text{ s}^{-1} \cdot \text{T}^{-1}$$

$$\frac{\gamma(^1\text{H})}{\gamma(^{13}\text{C})} \approx 4$$

But, we also need to factor in the % of isotope in natural abundance:

Isotope	% NA	γ (10^6)
^1H	100	267.522
^{13}C	1.11	67,283
^{19}F	100	251.815
^{31}P	100	108.394
^{11}B	20	28.747
^{10}B	80	85.84

- Compare the combined influence of γ & NA. For ^1H & ^{13}C

$$\frac{\gamma(^1\text{H})}{\gamma(^{13}\text{C})} = 4 \quad ; \quad \frac{\text{NA}(^1\text{H})}{\text{NA}(^{13}\text{C})} = 100$$

Receptivity

- The strength of the NMR signal:

$$S_{\max} \propto |\gamma^3 N|$$

nuclei

- The relative receptivity for $^1\text{H}/^{13}\text{C}$ is:

$$\begin{aligned} - \frac{S_{\max}(^1\text{H})}{S_{\max}(^{13}\text{C})} &= \frac{\gamma_{^1\text{H}}^3 N_{^1\text{H}}}{\gamma_{^{13}\text{C}} N_{^{13}\text{C}}} \\ &= (4)^3 (100) \\ &= 6400 \end{aligned}$$

Now we reconsider polarization, N_α vs N_β

At 500 MHz (^1H), aka $\sim 11.74 \text{ T}$

$$\frac{N_\beta}{N_\alpha} = \exp \left\{ \frac{-\hbar \gamma B_0}{k_B T} \right\}$$

$$= \exp \left\{ \frac{-(1.0546 \times 10^{-34} \text{ J}\cdot\text{s}^{-1}) (267.522 \times 10^6 \text{ s}^{-1}\cdot\text{T}^{-1}) (11.74 \text{ T})}{(1.3805 \times 10^{-23} \text{ J}\cdot\text{K}^{-1}) (298 \text{ K})} \right\}$$

$$= \exp \left\{ -8.051 \times 10^{-5} \right\}$$

$$\approx 0.99992$$

So, for every 100,000 spins (^1H nuclei)...

$$\frac{N_\beta}{N_\alpha} = 0.99992 ; N_\beta = (0.99992) N_\alpha$$

$$N_\alpha + N_\beta = 100,000 ; N_\alpha + (0.99992) N_\alpha = 10^5$$

$$(1.99992) N_\alpha = 10^5 ; N_\alpha = 50002$$

$$N_\beta = 100,000 - N_\alpha = 49998$$

$$N_\alpha - N_\beta = 4$$

S_0 , @ 11.74 T (500 MHz ^1H):

- Only 4 spins per 10^5 are net
- We need a lot of spins!
- In 0.8 mL of say H_2O there are

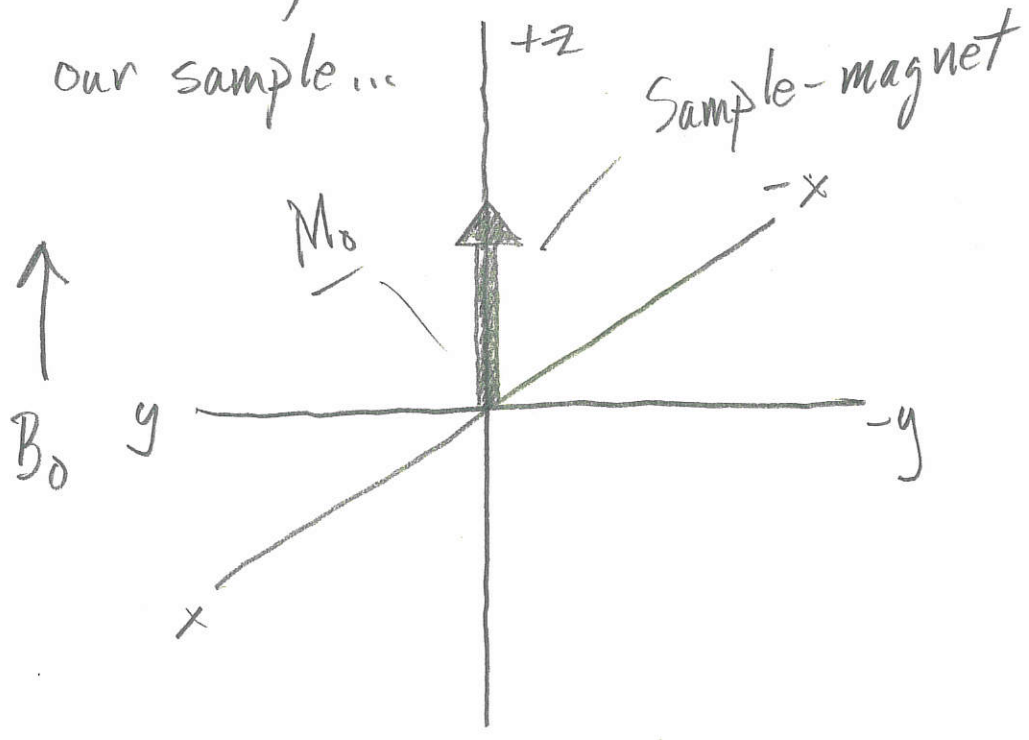
$$\rho_{\text{H}_2\text{O}} \cdot V$$

$$\left(\frac{1\text{g}}{1\text{mL}}\right)(0.8\text{mL}) = 0.8\text{g}$$

$$\# \text{ mol } \text{H}_2\text{O} = \frac{0.8\text{g}}{18\text{g/mol}} = 0.028 \text{ mol}$$

$$\begin{aligned} \# \text{ molecules } &= N_A(0.028 \text{ mol}) \\ \text{H}_2\text{O} &= (6.022 \times 10^{23} \text{ mol}^{-1})(0.028 \text{ mol}) \\ &= 1.67 \times 10^{22} \end{aligned}$$

- Now then, sometime after we introduce our sample ...



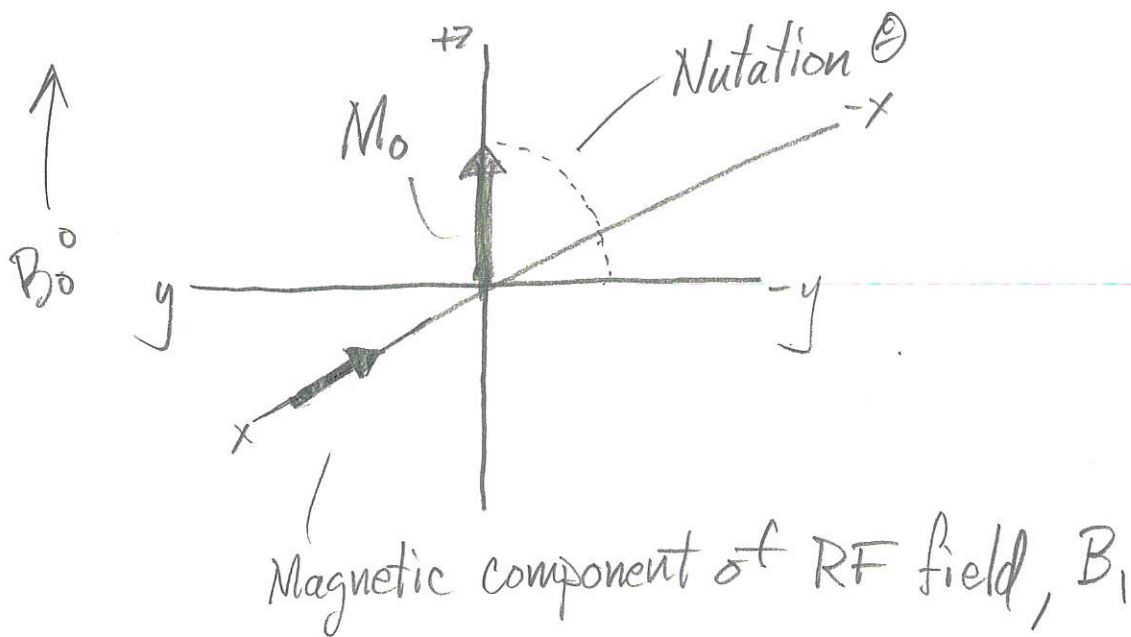
- Our sample is now a magnet!
- The phenomenon described above was named by our hero Felix Bloch, Nuclear Induction

F. Bloch
 b. 1905
 d. 1983
 ETHZ (Dobner & Weyl)
 PhD (Heisenberg, Leipzig)

- The remainder of NMR technology, more or less, is concerned with perturbation or the induced nuclear magnetism.

- Most basic experiment:

Nutation - Detection of Free Precession



- The magnetic component of an applied radio-frequency (RF) field exerts a torque on M_0 , causing nutation of M_0 in the direction of the $-y$ -axis as predicted by the standard interpretation of the right-hand-rule...
- Non-standard right-hand-rule?!

$$\underbrace{\frac{d\vec{M}}{dt}}_{\substack{\text{Rate} \\ \text{of} \\ \text{Change}}} = \underbrace{\vec{M} \times \gamma \vec{B}_1}_{\text{Torque}}$$

- The nutation- θ thus depends on:
 - 1) The intensity of the magnetic component of the applied RF field, B_1
 - 2) The gyromagnetic ratio of the spins
 - 3) The duration during which the RF is applied

- Rotation of a magnetic moment around an applied magnetic field is predicted by the Larmor Theorem:

$$\vec{\omega} = -\gamma \vec{B}$$

- The nutation angle is

$$\theta = \tau_p \gamma B_1$$

- Thus, given a particular spin, e.g. ¹H, and a constant value for B₁, the nutation angle increases linearly with time.

- A characteristic parameter NMR instruments is the τ_p such that θ = π/2 (90°)

- Consider ¹H : 10 μs ^{τ_p(90°)} RF duration (pulse!) ↓

$$\frac{\pi}{2} = (10^{-6} \text{ s}) (267.522 \times 10^6 \text{ s}^{-1} \cdot \text{T}^{-1}) B_1$$

$$B_1 = \frac{(1.5708)}{267.522 \cdot \text{T}^{-1}}$$

$$B_1 = 5.872 \times 10^{-3} \text{ T}$$

$$= 58.72 \text{ G } \left\{ \begin{array}{l} \times 100 \text{ B of Earth!} \end{array} \right. \uparrow$$