

## Solutions

1(a)  $I = 3/2$ . Number of levels is  $(2I+1) = 4$

1(b) One would expect to see only one line as the energy levels are all equally spaced.

1(c) Use the Larmor equation and solve for  $B_0$ .

$$\begin{aligned} B_0 &= (2\pi\nu)/\gamma \\ &= 2 * (\pi \text{ rad}) * (1.92546 \cdot 10^8 \text{ sec}^{-1}) / (8.5843 \cdot 10^7 \text{ rad T}^{-1} \text{ sec}^{-1}) \\ &= 14.093 \text{ T} \end{aligned}$$

1(d)  $\nu_H = \nu_B(\gamma_H/\gamma_B)$

$$\begin{aligned} &= (1.92546 \cdot 10^8 \text{ sec}^{-1}) * (2.67519 \cdot 10^8 \text{ rad T}^{-1} \text{ sec}^{-1} / 8.5843 \cdot 10^7 \text{ rad T}^{-1} \text{ sec}^{-1}) \\ &= 6.00046 \cdot 10^8 \text{ sec}^{-1} \\ &= 600.046 \text{ MHz} \end{aligned}$$

2. INOVA 400 means that the  $^1\text{H}$  resonance is at at 400 MHz

$$\begin{aligned} \nu_C &= \nu_H(\gamma_C/\gamma_H) \\ &= 400 \text{ MHz} (6.7283 \cdot 10^7 \text{ rad T}^{-1} \text{ sec}^{-1} / 2.67519 \cdot 10^8 \text{ rad T}^{-1} \text{ sec}^{-1}) \\ &= 100.60 \text{ MHz} \end{aligned}$$

1 ppm for  $^{13}\text{C}$  is therefore  $1 \cdot 10^{-6} * 1.0060 \cdot 10^8 \text{ Hz} = 100.60 \text{ Hz}$

The difference between the lines was 11,559.26 Hz.

In ppm this is  $11,559.26 \text{ Hz} / 100.60 \text{ Hz/ppm} = 114.9 \text{ ppm}$

The chemical shift of the aromatic carbons is therefore  $17.3 \text{ ppm} + 114.90 \text{ ppm}$

$$= 132.2 \text{ ppm}$$

3. When the signal is on-resonance, it is in the center of the excitation profile of the pulse.

When it is significantly off-resonance, the signal is closer to the edge of the excitation profile of the pulse and therefore is not excited to the same extent. As a result its intensity is not as high as that measured when it is on-resonance.

4.  $270^\circ = 6.5 \mu\text{s}$ ,  $360^\circ = 8.5 \mu\text{s}$ ,  $180^\circ = 4.5 \mu\text{s}$ ,  $90^\circ = 2.5 \mu\text{s}$ .

5(a) From the diagram the signal has 10 period in one second therefore the frequency in the FID is 10 Hz. This means that the NMR signal is 10 Hz away from the carrier frequency.

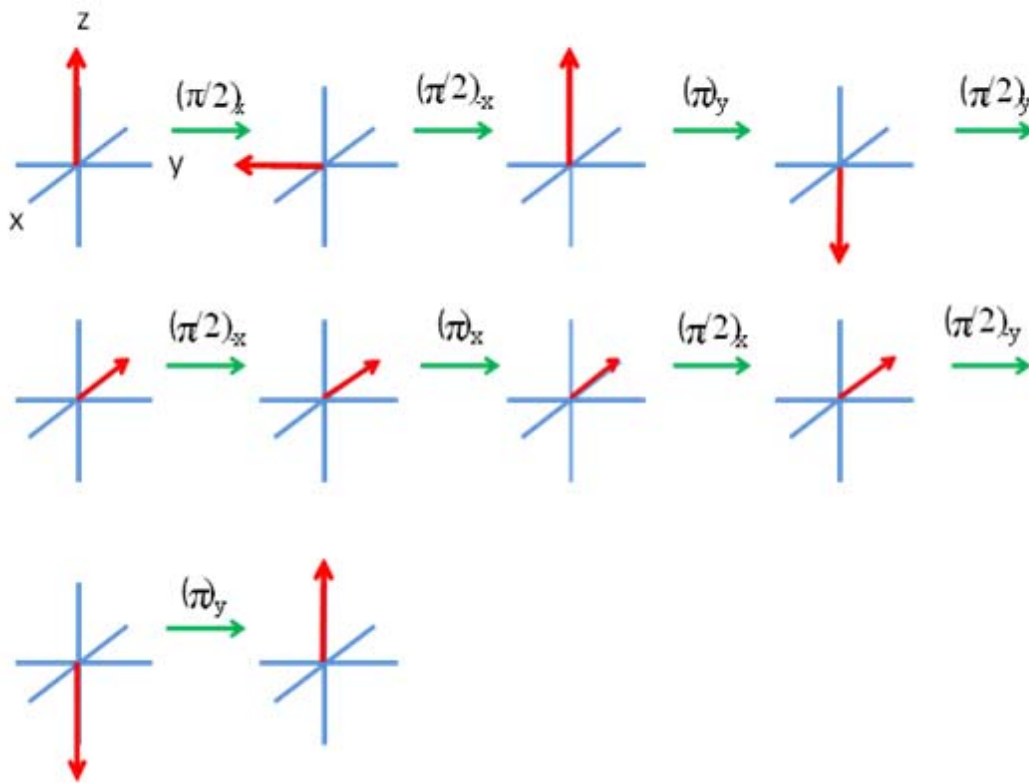
$$\begin{aligned} \nu_{Li} &= \nu_H(\gamma_{Li}/\gamma_H) \\ &= 600 \text{ MHz} (1.03975 \cdot 10^8 \text{ rad T}^{-1} \text{ sec}^{-1} / 2.67519 \cdot 10^8 \text{ rad T}^{-1} \text{ sec}^{-1}) \\ &= 233.198 \text{ MHz} \end{aligned}$$

Therefore 1 ppm = 233.198 Hz

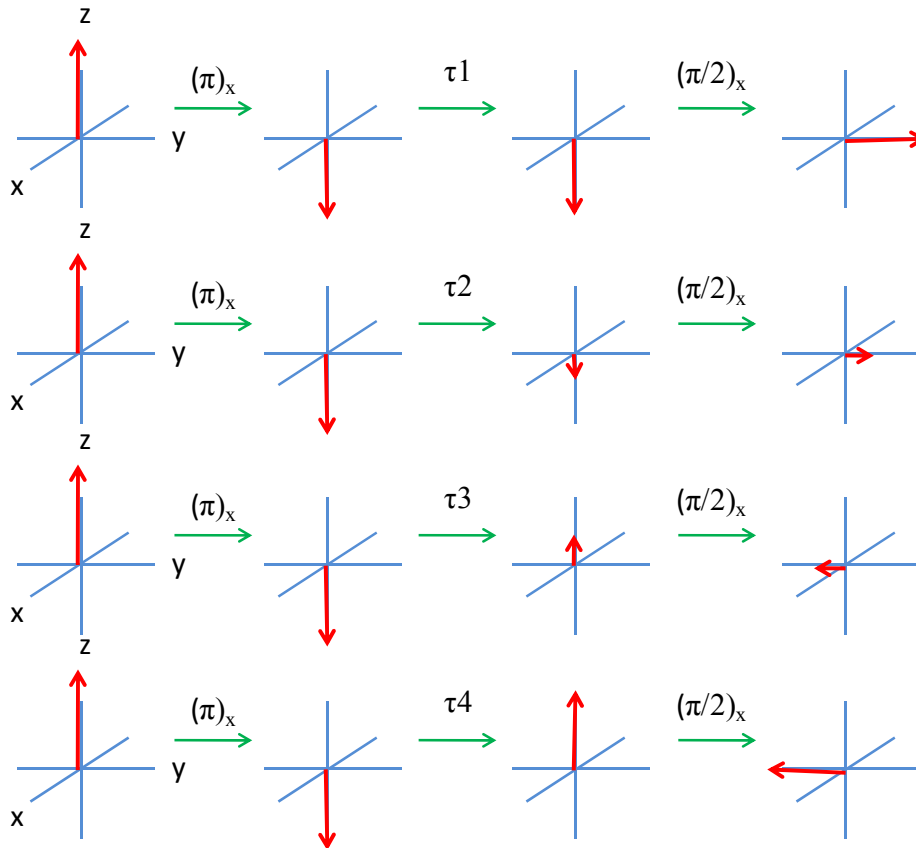
$$10 \text{ Hz} / 233.198 \text{ (Hz/ppm)} = 0.0429 \text{ ppm}$$

5(b) A simple exponential decay (i.e. no oscillations) with the same overall decay rate as the FID shown.

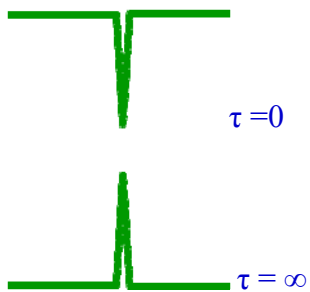
6. The magnetization resides on the z axis



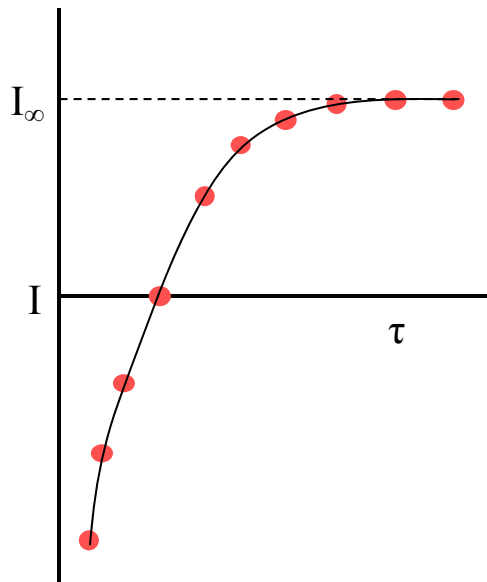
7(a)



7(b)



7(c)



7(d)  $T_1$

8. All of the NMR frequencies get mixed down to an intermediate frequency chosen by the instrument manufacturer. This frequency is chosen to optimize the performance of the electronics.

9(a)  $\Delta\nu = (\gamma/2\pi) \Delta B_0$

$$\Delta B_0 = \Delta\nu (2\pi/\gamma)$$

$$= (5.001399742 \cdot 10^8 \text{ Hz} - 5.001149352 \cdot 10^8 \text{ Hz})(2\pi \text{ rad} / 2.67519 \cdot 10^8 \text{ rad T}^{-1} \text{ sec}^{-1})$$

$$= 5.88087 \cdot 10^{-4} \text{ T}$$

9(b) One would have to introduce more current to the main coil of the magnet.

9(c) The frequency dropped by  $(5.001399742 \cdot 10^8 \text{ Hz} - 5.001149352 \cdot 10^8 \text{ Hz})$  in 20 years.

$$= 25039 \text{ Hz in 20 years}$$

$$25039 \text{ Hz} / 20 \text{ years} = 5.001399742 \cdot 10^8 \text{ Hz} / X \text{ years}$$

$$X = 399,489 \text{ years}$$

$$10. (\text{relaxation delay} + \text{pulse} + \text{acquisition time}) * 4096 = 4.5 \text{ hours}$$

$$\text{Each scan took } (4.5 \text{ hours} * 3600 \text{ sce/hour}) / 4096 = 3.955 \text{ seconds}$$

The pulse is negligible with respect to the relaxation delay and acquisition time and can therefore be ignored.

The relaxation delay was therefore  $3.955 \text{ seconds} - 1 \text{ second} = 2.955 \text{ seconds}$ .