Nuclear Magnetic Resonance

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Where Success Begins

Motivation

- The nuclear magnetic resonance concept is applied in NMR spectroscopy
- NMR spectroscopy is used for chemical identification and analysis, as well as imaging, in both biological and non-biological system

NMR Theory

Spin & Magnetic Moment

- Spin is a fundamental property of fermions (protons and neutrons)
- Spin comes in multiples of ½, and produces magnetic moment, which is either parallel (+½) or anti-parallel (-½) when exposed to static magnetic field ($\vec{B_0}$), if net spin is ½
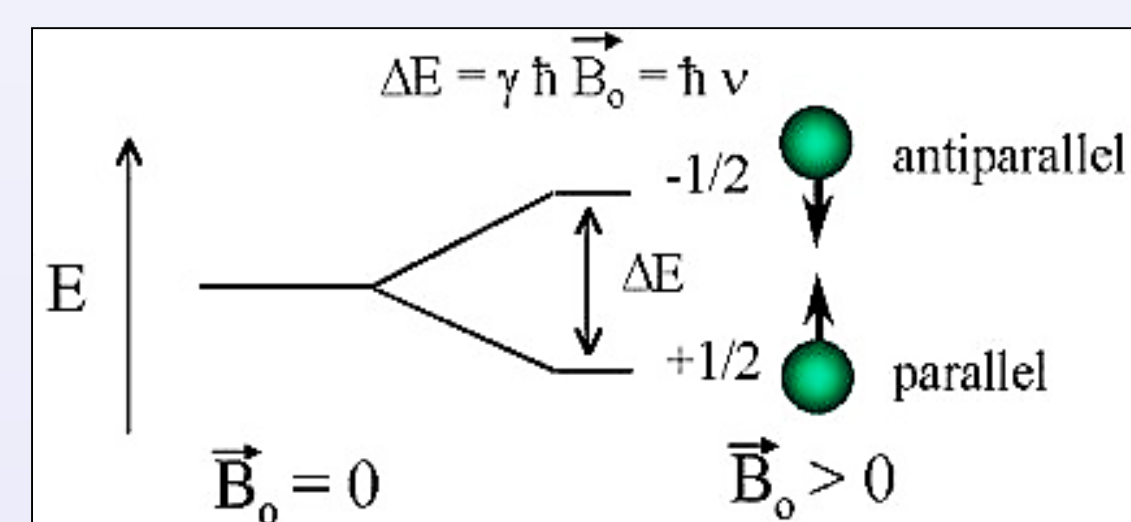

Fig 1. Two states of spin, orientation, and its energy level relative to each other

- Net spin will not be observed if the +½ and -½ spin particles area equal in quantity
- The population ratio of the two spin states is proportional to the Boltzmann statistics

$$\frac{N1\ (anti-parallel)}{N2\ (parallel)} \propto e^{\frac{E2-E1}{kT}}$$

Alignment and Precession

- The potential energy of a magnetic dipole is given by

$$E = -\vec{\mu} \cdot \vec{B} = -\mu B cos(\theta)$$

- To minimize energy (E), θ must be 0, which means the magnetic moment (μ) is aligned with the field ($\vec{B_0}$)
- However, perfect alignment can only happen at absolute zero. At any other temperatures, the nuclei will not be exactly aligned with the magnetic field
- Due to its angular momentum, the direction of the magnetic moment rotates around the magnetic field direction. This is called precession.

Alignment and Precession

- Nuclei will precess at a certain Larmor frequency, represented by the equation

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

- $\vec{\omega}$ is the Larmor frequency and γ is the gyromagnetic ratio
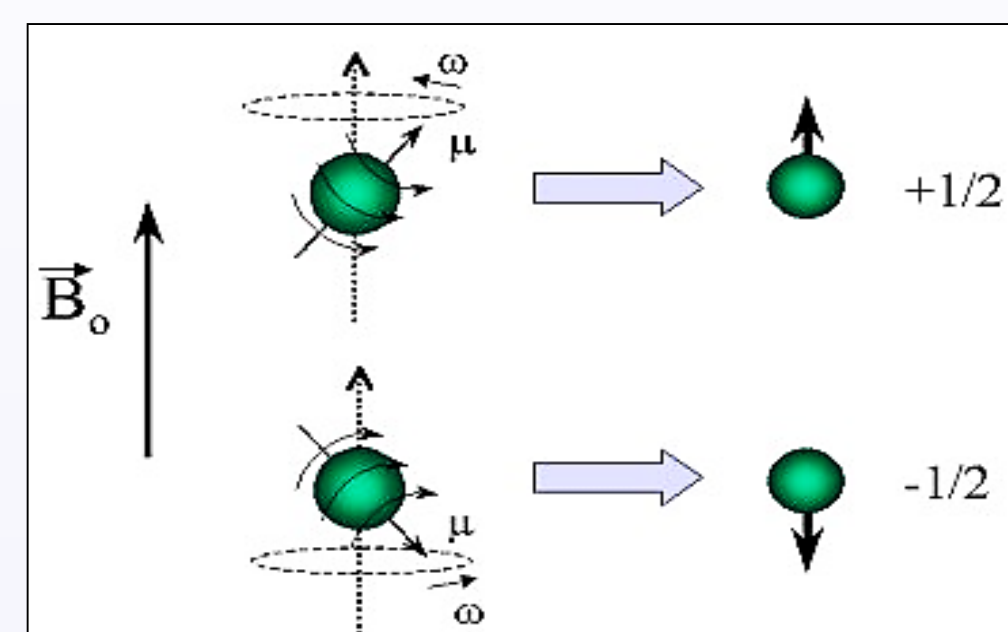

Fig 2. Precession of nuclei under a magnetic field $\vec{B_0}$

T1, T2, and Rf Processes in NMR Spectroscopy

- The first T1 process (spin lattice relaxation) is when an external static magnetic field is introduced
- Radiofrequency signal is generated by passing an electric current through the NMR coil
- If the frequency of the Rf signal is very similar to the Larmor frequency of the nuclei, resonance happens
- During resonance, in this case, proton will absorb the electromagnetic radiation and start rotating to a higher energy spin state.
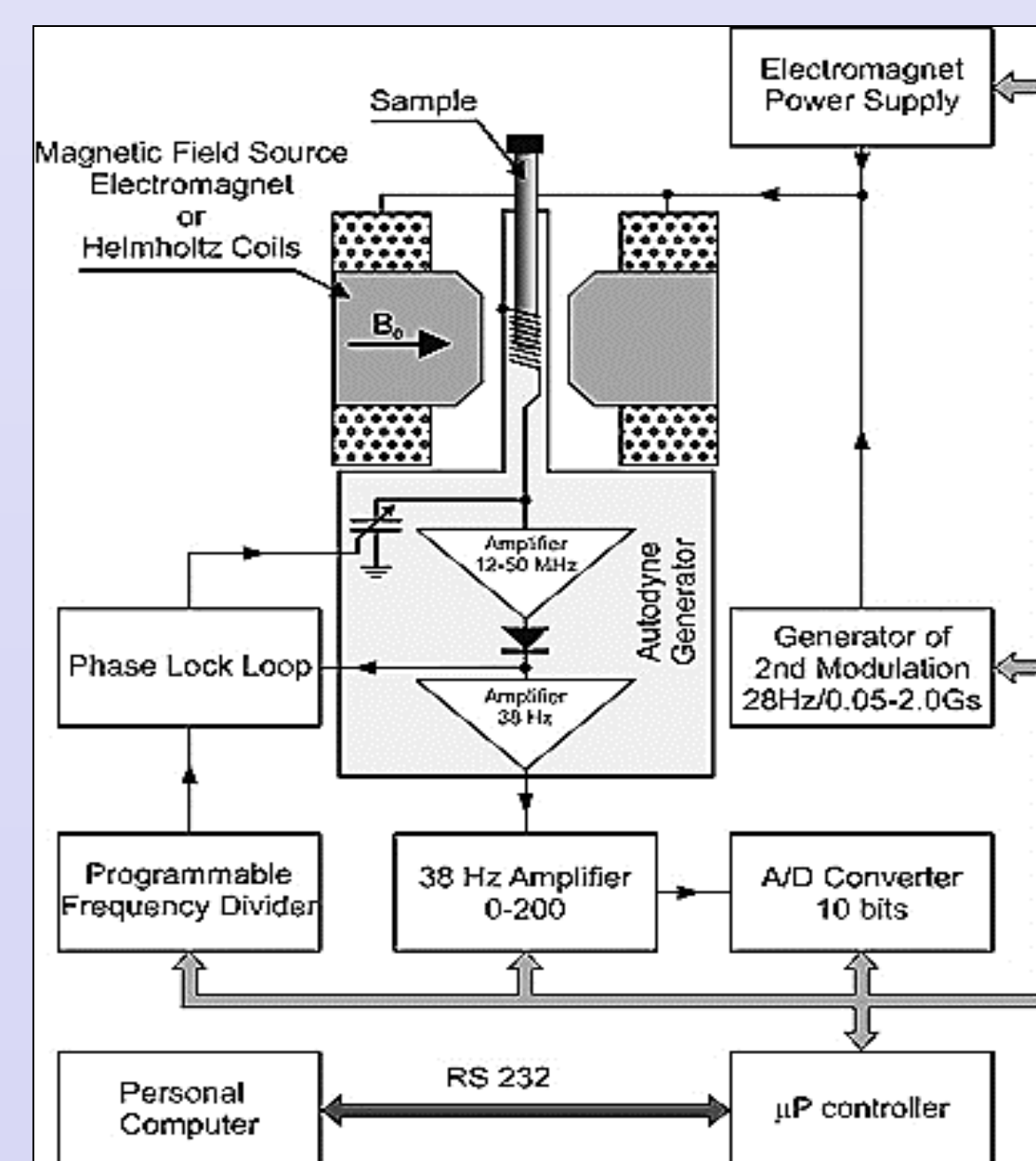- NMR spectrometer usually uses 90 degrees Rf signal (function of time) to be useful.

Fig 3. Components of NMR Spectroscopy. Note that the NMR coil is perpendicular to the direction of $\vec{B_0}$

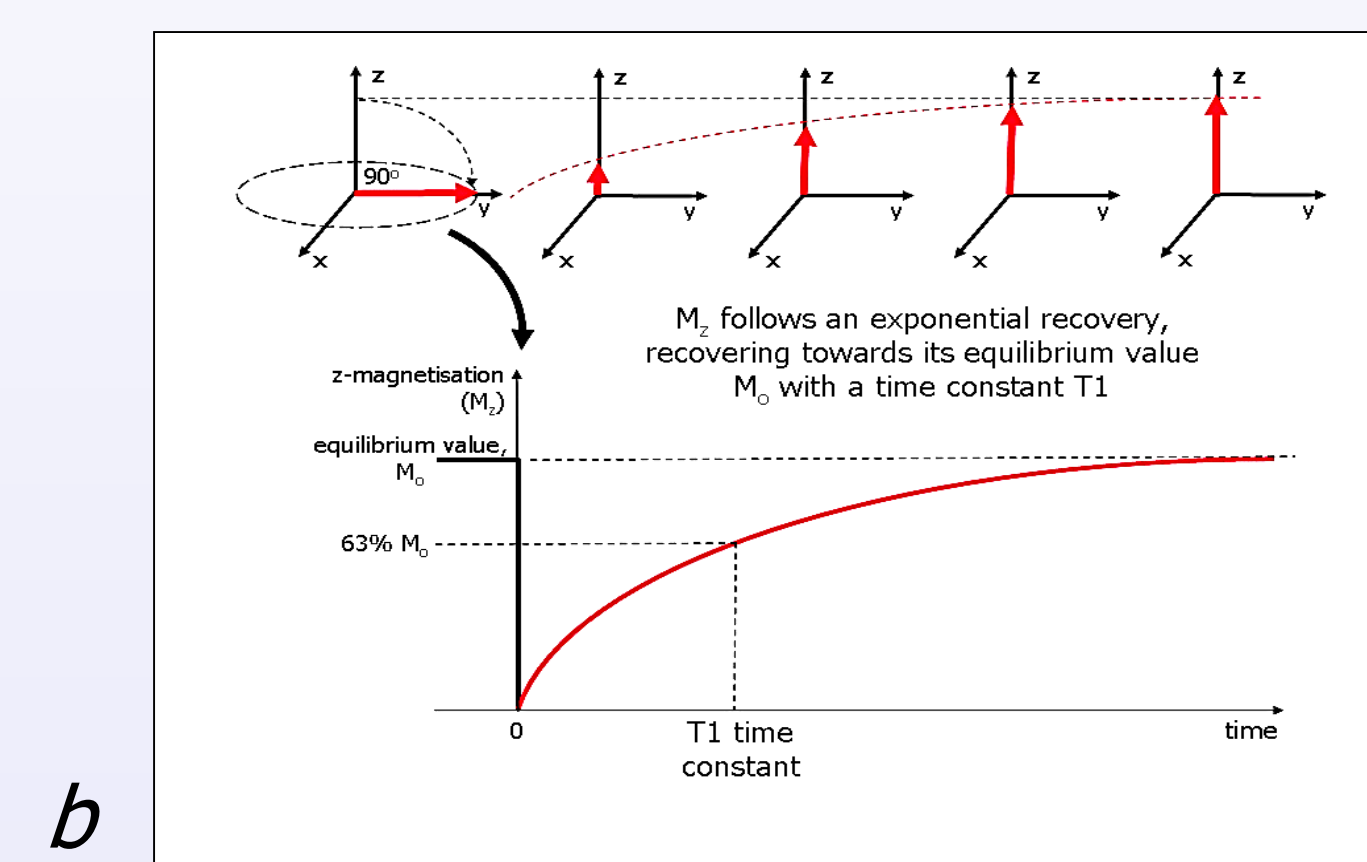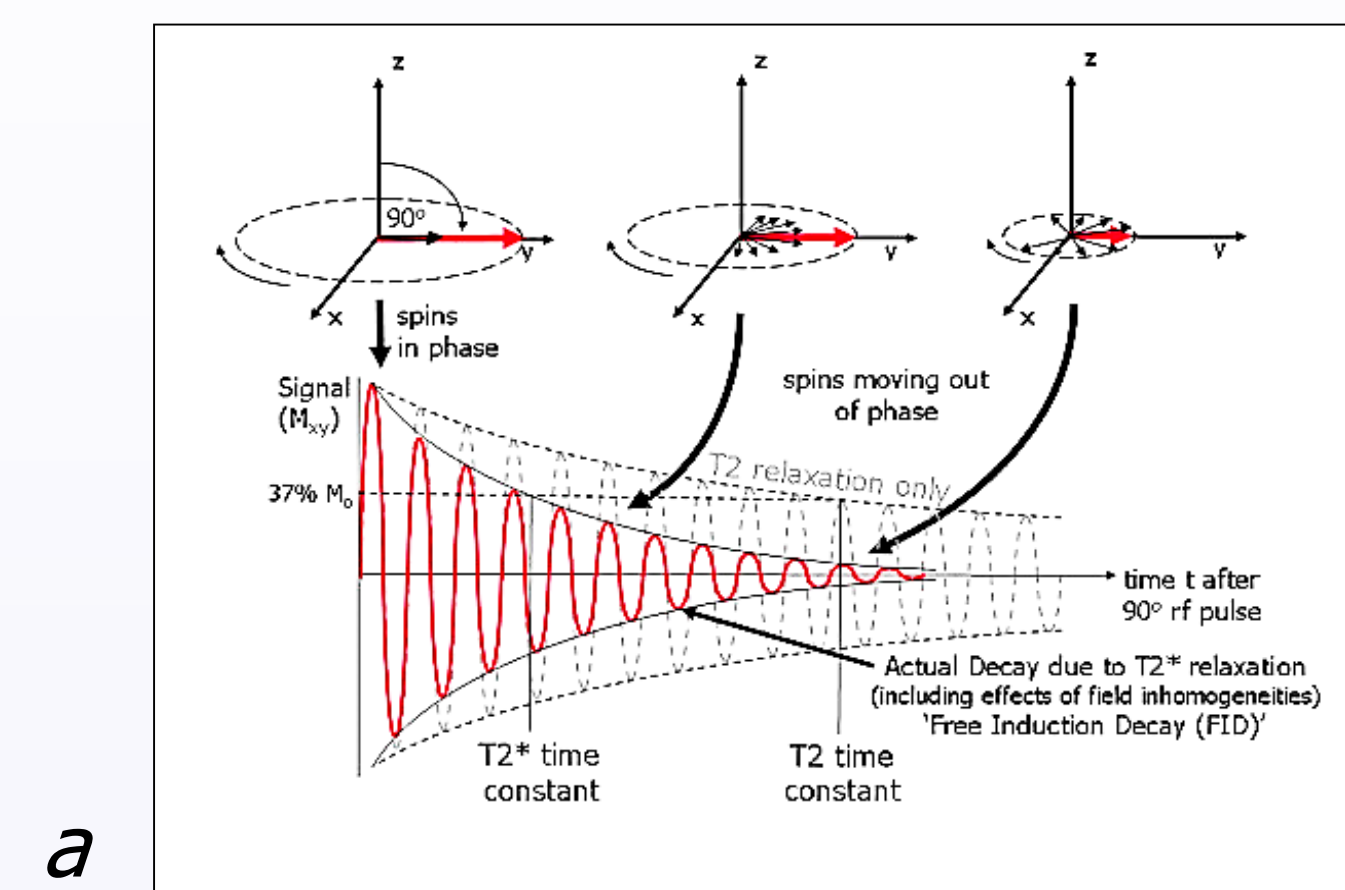## T1, T2, and Rf Processes in NMR Spectroscopy

a

b

Fig 4. (a) T2 and T2* processes with the FID graph . (b) T1 process & the recovery graph

- After the Rf signal is turned off, the nuclei will try to return to its earlier thermodynamically stable spin state
- Due to the magnetic field inhomogeneity and diamagnetic shielding, the protons are each precessing at a slightly different resonance frequency
- This causes decoherence of tranverse/x-y magnetization (T2 & T2* spin-spin relaxation)
- T1 process also happens simultaneously, reverting the spin back to its thermodynamically stable state
- Since magnetic field is changing, magnetic flux (ϕ) is changing over time and this induces voltage (ε) per Faraday's Law in the NMR coil

$$\phi_B = \iint_{\Sigma(t)} \vec{B}(r,t) \cdot \vec{dA}$$

$$\varepsilon = -\frac{d\phi_B}{dt}$$

- The voltage induced is amplified and recorded as the Free Induction Decay graph (see figure)

FID, Fourier Transform, & NMR Spectrum

- After FID graph is obtained, Fourier Transform method is used to convert function of time to function of frequency (NMR spectrum)
- This is done by deconstructing the FID graph into more sinusoidal functions
- NMR spectrum is used by scientists to determine molecular structure

$$F(\omega) = c \int_{-\infty}^{\infty} f(t)\, e^{-is\omega t}\, dt$$
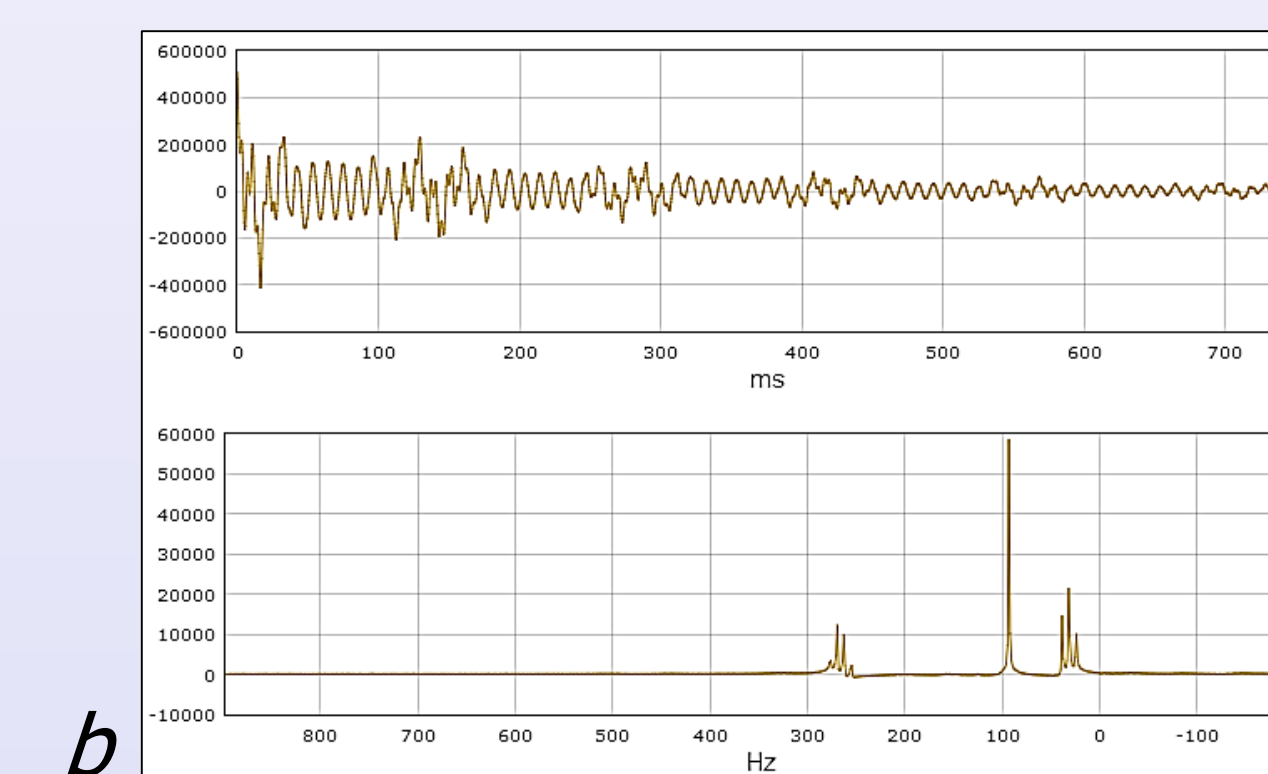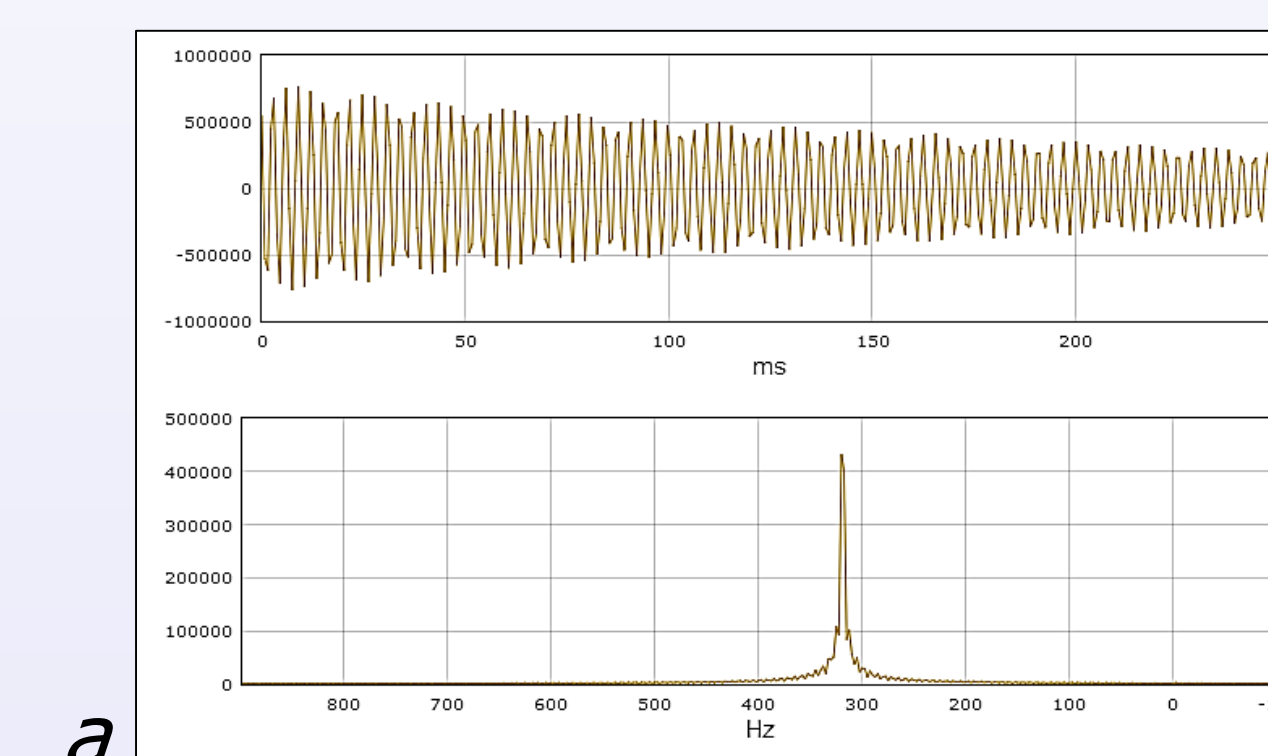
FOURIER TRANSFORM

a

b

Fig 5. FID and NMR spectrum of: (a) Deionized Water, H_2O and (b) Ethyl acetate, EtOAc. Figures taken from LCC's PicoSpin 80 NMR

References

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Fig 1 & 2:
NMR Lectures (n.d.). In *The University of Maine, Department of Chemistry*. Retrieved April 15, 2014, from http://chemistry.umeche.maine.edu/CHY431/NMR/NMR-3.html

Fig 3:
Spin Resonance (n.d.). In *TEL-Atomic*. Retrieved April 17, 2014, http://www. telatomic.com/images/spin_resonance/nmresr_blockdiagra m.gif

Fig 4a:
Transverse (T2 and T2*) relaxation processes (n.d.). In *Journal of Cardiovascular Magnetic Resonance*. Retrieved April 15, 2014, from online.com/content/12/1/71/figure/F4http://www.jcmr-

Fig 4b:
T1 relaxation processes (n.d.). In *Journal of Cardiovascular Magnetic Resonance*. Retrieved April 15, 2014, from http://www.jcmr-online.com/content/12/1/71/figure/F3?highres=y

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