NMR Short Course 2010

Problem Set I

Read:
Chapter 2 --- *High Resolution NMR Techniques in Organic Chemistry*

1. Natural carbon (Z = 6) is composed of two isotopes, ^{12}C and ^{13}C. The atomic mass listed for carbon in the periodic table is 12.01. (1) What is the composition of each nucleus? (2) What is the natural abundance of each isotope? Note: General question for Chemistry

2. What is the energy difference between the two spin states of ^{1}H in magnetic field of 9.395 Tesla (400MHz instrument) and 18.79 Tesla (800MHz instrument), How about ^{13}C? ($\gamma_H = 267.512 \times 10^6$ rad T^{-1} S^{-1} and ($\gamma_C = 67.2640 \times 10^6$ rad T^{-1} S^{-1}). How much intensity will increase by using 800 MHz instrument, instead of using 400 MHz instrument. Note: Read book page 12.

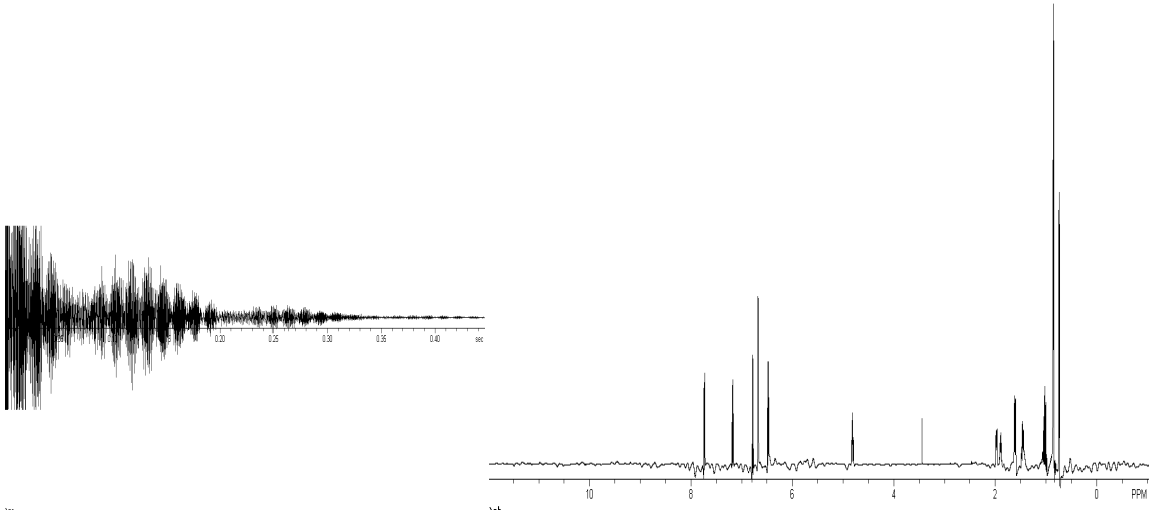
$$\Delta E = \frac{\gamma \hbar B}{2\pi}$$

3. (1). At 20 ^{0}C what fraction of ^{1}H nuclei in 9.395 T field are the upper and lower states? (2). of ^{13}C? Note: read book page 12-13.

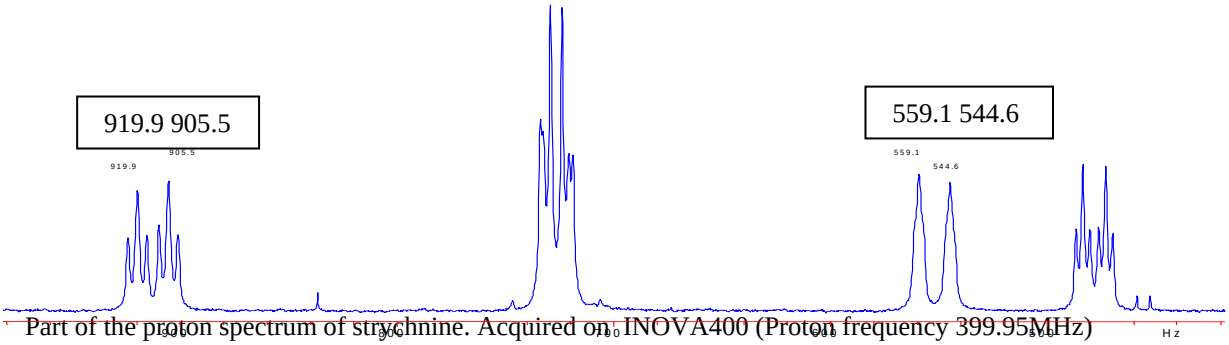
4. (a). Suppose that for a certain set of ^{13}C nuclei at 25°C, the value of T_1 is 2 s. How long after immersion in a 9.395 Tesla magnetic field will it take for an initially equal distribution of ^{13}C spin states to progress 95% of the way toward equilibrium? (b). What would happen if the magnet were turned off at this point? Note: Read "High-Resolution NMR Techniques in Organic Chemistry" page 21 section 2.4.1

5. Explain what effect dissolved Oxygen (O_2) might have on longitudinal relaxation of ^1H nuclei. *Hint: the oxygen molecule has two unpaired electrons with the same s value.* Note: General chemistry Question.

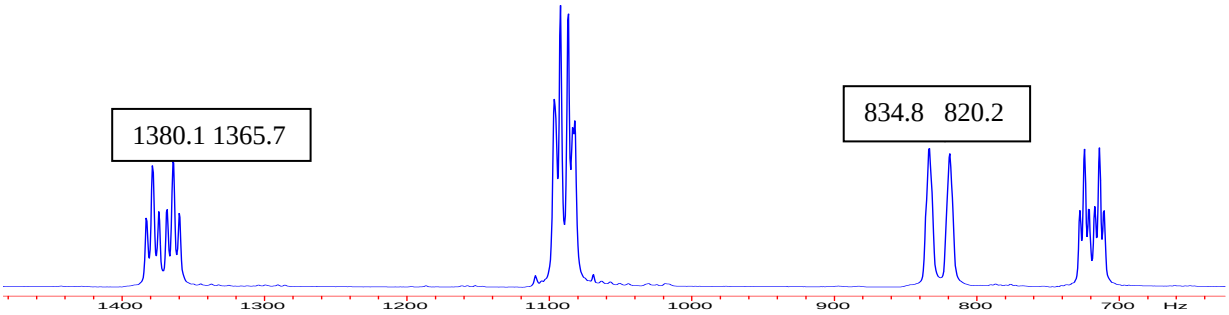
6. The following spectrum was acquired on our INOVA400. Explain what is happened and to change which parameters will make the spectrum better? Note: Read book. Page 51.



6. Following two ^{1}H spectra of strychnine acquired on INOVA400 and INOVA600. (1). Calculate the chemical shifts of four labeled signals from both instruments. (2) Calculate the homonuclear J coupling of two protons using the data on the spectra.



Part of the proton spectrum of strychnine. Acquired on INOVA400 (Proton frequency 399.95MHz)



Part of the proton spectrum of strychnine. Acquired on INOVA600 (Proton frequency 599.64MHz)
835.0 820.2