

PROBLEM SET 2 BCMB/CHEM 8190

1) It is frequently important to know the rf field imposed by a spin decoupling coil in an NMR experiment. Suppose we use the decoupling coil to provide a proton excitation pulse and determine that we need to apply rf for 200 μ s to get a 90 degree pulse. What is the rf field in Tesla?

2) Sometimes you may not want to excite a certain resonance (i.e. a water resonance in an aqueous sample). Suppose this resonance was 1000Hz away from your rf frequency. Sketch in magnetization vector diagrams qualitatively what would happen if a long 90 degree pulse (1 ms) and chemical shift offset simultaneously affected the resonance. PJ-NMR (as used in the Friday Lab section) can apply rotation operators representing small increments of rf and chemical shift to simulate this more accurately. Could you use it to find a combination of rf and shift offset that results in no observable transverse magnetization for the resonance?

2 We build an NMR probe based on a parallel LC circuit with $L = 8$ micro Henries and $C = 0.3$ pF. At what frequency does it resonate? What is the Q of the coil assuming 10 Ohm resistance? What is the decay constant for current in the coil?

4) We measure the width of a Lorentzian line in an NMR spectrum to be 2 Hz. If this line width is totally dictated by spin relaxation, what is the T_2 for the site? If one Hz is contributed by magnet inhomogeneity, what is the T_2 ? If we multiplied the FID before Fourier transformation by an exponential with decay constant of 1 s and the inhomogeneity contribution is 1 Hz, what is the T_2 .

5) You are going to acquire a ^{13}C spectrum of a compound with a 5 sec T_1 and 0.3 sec T_2 for most carbons. You anticipate resonances over a 200 ppm region at 50 MHz. What values for the following acquisition and processing parameters would you choose in order to optimize signal to noise with minimal sacrifice in spectral resolution and dispersion:

- a) acquisition time
- b) number of time domain points
- c) pulse angle
- d) delay between acquisitions
- e) line broadening