BCMB/CHEM 8190
ANSWERS TO PROBLEM SET 1

1) Receptivities are given in the table relative to ^{1}H (and also relative to ^{13}C). Relative to ^{1}H, these are proportional to the ratios of γ^3, then correcting for natural isotopic abundance.

receptivity for $^{13}C = \gamma^3_{13C} / \gamma^3_{1H} \times$ natural isotopic abundance of ^{13}C
$= (6.7283 \times 10^{-7})^3/(26.7522 \times 10^{-7})^3 \times 0.011 = 1.75 \times 10^{-4}$

Divide by abundance to get receptivity for equal number of nuclei (i.e. don't include correction for natural isotopic abundance……this is relative sensitivity)

The frequencies depend linearly on γ.

Receptivity dependence on γ can be seen by equating the ratio of the γ values raised to some power, n, comparing to the receptivity of an equal number of nuclei and finding n (you'll find n=3)

Receptivity also is proportional to 1/T. Therefore at 4 versus 300K the relative receptivity is 75 times larger.

2) The difference in precession frequency is:
$[(26.7522 \times 10^7$ rad/T/s$) \times 11.7$ T $\times (60-55.2) \times 10^{-6}]/2\pi$, or 2391Hz.
The methyl resonance is 4.8 ppm upfield of the OH resonance.

3) The best way to approach this problem is to fit the data to the equation given in class ($M_z=M_0(1-2e^{(-t/T1)})$), or, more appropriately, $I_z=I_0(1-2e^{(-t/T1)})$).

Another way to approach this problem is to linearize the equation we gave in class and either graph the data, or use your favorite linear least squares program. The equation after rearranging and taking the log of both sides is: $\ln((I_0-I)/I_0) = \ln(2) - t/T_1$. Plotting and taking the slope of the best line to be $1/T_1$ we get a T_1 of about 4.1s.

A good way to estimate the value is to make your best estimate for the time when the signal is zero, solve the equation for the time when I=0 ($T_1=t/\ln(2)$).

4) $\omega = -\gamma B_1$. If $t \times \omega = -\pi/2$, $B_1 = 1/t \times \pi/2 \times 1/\gamma = 2.94 \times 10^{-5}$ T