

BCMB/CHEM 8190
PROBLEM SET 3

- 1) Write down a Hamiltonian for a pair of spin 1/2 spins in a static B_0 field using the z component spin operators I_{z1} , I_{z2} , their coupling constant J_{12} , and their chemical shieldings, σ_1 and σ_2 . Make an energy level diagram showing the positions of levels for the four simple product spin functions. Show the allowed one quantum transitions and calculate the energy differences associated with them. Sketch and label the corresponding lines in a frequency resolved spectrum.

- 2) Write down the operator for the total z magnetization for a two spin 1/2 system in terms of the single spin operators (call the spins 1 and 2). Evaluate the magnetization (expectation value) associated with the alpha/alpha and alpha/beta spin states. What is the expectation value for the total I^2 operator for these two states? What is the expectation value for the z magnetization of spin 1 in these two states?

- 3) Couplings between 5' and 5'' protons and the phosphate phosphorus in a 5' nucleotide are observed to be 6.0 and 8.0 Hz, respectively. Using the formula $J(\text{PH}) = 21(\cos(\theta))^2 - 2.25$, and assuming idealized rotamer geometries about the C5 - O5 bond, calculate the rotamer populations for this molecule.