Chemistry 988 Section 2
Second Problem Assignment (due Monday, March 15, 1999 in class)

1. Explain each phenomenom in a few sentences:

   (a) chemical shift anisotropy
   (b) quadrupolar coupling
   (c) nuclear dipole coupling
   (d) J-coupling

   How does the nuclear dipole coupling depend on internuclear distance?

2. The quantum mechanical expression for dipolar coupling energy between two different nuclei I and S in a strong magnetic field:

$$(\mu_0/4\pi)(h^2\gamma_I\gamma_S/4\pi^2r^3)(1-3\cos^2\theta)I_zS_z$$

where I_z and S_z correspond to the z components of the nuclear spin for nuclei I and S, respectively, r is the internuclear distance, θ is the angle between the internuclear vector and the magnetic field axis, and μ_0 is the 'permeability of free space'. The value for μ_0 is 4π X 10^{-7} kg-m/(s^2-A^2).

Calculate the dipolar energy/h (i.e. frequency) for each of the six possible combinations of nuclear spin states in a directly bonded ^{13}C-^{14}N pair in a peptide bond. You should use r = 1.32 Å and $\theta = 90°$.

Repeat the calculation for $\theta = 54.7356°$.

3. Consider the solid state NMR ^{13}C spectra of C_{60} from Figure 2 of the attached paper, Phys. Rev. Lett., **67**, 1886-1889 (1991).

Explain in a few sentences the observed temperature dependence of the spectral linewidths and lineshapes.