Chemistry 474b
Problem Set #1 (Due in class: Monday January 22, 2007)

This problem set is designed to refresh your C374a memory. Where appropriate use SI units. Feel free to look up any integrals you may need!

1.) Express the quantum mechanical operator for the following function f in its most explicit form:

$$f = xp_y^2 + e^{-t^2} + \sqrt{y}\,p_x p_z^2$$

2.) An extremely crude picture of an electron in an atom or molecule treats it as a particle in a one-dimensional box whose length is on the order of the size of atoms and molecules.
a) For an electron in a one dimensional box of length 1.0 Å, calculate the separation between the two lowest energy levels.
b) Calculate the wavelength of a photon corresponding to a transition between these two levels.
c) In what portion of the electromagnetic spectrum is this wavelength?

3.) At time zero a linear harmonic oscillator is in a state that is described by the following normalized wave function:

$$\psi(x) = \sqrt{\frac{1}{5}}u_0(x) + \sqrt{\frac{1}{2}}u_2(x) + c_3u_3(x)$$

where $u_n(x)$ is the nth time independent eigenfunction for the oscillator.
a) Determine the numerical value of c_3 assuming it to be real and positive.
b) What is the expectation value of the energy of the oscillator at t = 0?

4.) Given a superposition stationary state wave function for a rigid rotor:

$$\Omega = \sqrt{\frac{1}{3}}Y_2^1 + \sqrt{\frac{1}{6}}Y_2^2 + \sqrt{\frac{1}{2}}Y_2^{-2}$$

a) What is the probability of finding the system in state $Y_2{}^1$?; in state $Y_2{}^2$?; in state $Y_2{}^{-2}$?; in a state $Y_\ell{}^m \neq Y_2{}^1$, $Y_2{}^2$, or $Y_2{}^{-2}$?

b) Write down the expectation value of $\hat{L}_z$ and $\hat{L}^2$ when the system is in state Ω.

Recall: $Y_\ell^m(\theta,\varphi)$ are the spherical harmonic functions.

5.) a) What are <r> and <1/r> for the 1s orbital of atomic hydrogen?
b) What is the transition dipole moment , -ez, in debye for the $2p_z \leftarrow 1s$ transition of hydrogen?
Note: 1 debeye, D =3.3346 x 10^{-30} C-m.