Core Course 2002
Homework Part II, Problem Set 2

1. a) In the example of formaldehyde discussed in class, we concluded that the n->π* transition was strictly forbidden. For formaldehyde, you can make a very simple argument that in fact, this is not strictly true. Symmetry dictates that the transition will not be completely forbidden. **Explain** (bring some of what you learned from the first half of the course; the conclusion *would* be true for ethylene).

   b) Reevaluate the integrals as we did in class, but now using your new understanding of formaldehyde. For single crystals of formaldehyde, predict whether light polarized along x, y, and z will induce each transition.

2. We have seen that quenching of fluorescence can depend on the concentration of the quenching agent. Assuming that quenching is first order with respect to the quencher Q (with a first order rate constant of k_q), derive an expression for the ratio of the fluorescence in the absence of quencher to that in the presence of quencher, F_o/F_Q, as a function of [Q], k_q, and τ_o (the lifetime of the excited state in the absence of quencher).

3. For the particle in a box problem,
   a) show that the following is an eigenfunction of H.

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$$

   b) show that this is a normalized wavefunction

Potentially useful equations:

$$\int \cos(ax)dx = \frac{\sin(ax)}{a}$$

$$\int x\cos(ax)dx = \frac{\cos(ax)}{a^2} + \frac{x\sin(ax)}{a}$$

$$\int x^2\cos(ax)dx = \frac{2x}{a^2}\cos(ax) + \left(\frac{x^2}{a} - \frac{2}{a^3}\right)\sin(ax)$$

$$\int \cos^2(ax)dx = \frac{x}{2} + \frac{\sin(2ax)}{4a}$$

$$\int \sin^2(ax)dx = \frac{x}{2} - \frac{\sin(2ax)}{4a}$$

$$\int x\cos^2(ax)dx = \frac{x^2}{4} + \frac{x\sin(2ax)}{4a} + \frac{\cos(2ax)}{8a^2}$$

$$\int x\sin^2(ax)dx = \frac{x^2}{4} - \frac{x\sin(2ax)}{4a} - \frac{\cos(2ax)}{8a^2}$$