Assignment #2

Recommended Problems (not to be handed in)
All of these problems are from McQuarrie & Simon.
Chapter 3: 1b, 1c, 3a, 3b, 6, 25, 32 (just read #32)
Math Chapter C:1, 4, 6, 7
Chapter 4: 4-14, 4-29 (just read #29)

Required Problems (Due Feb 28 at 3 pm)
1. McQuarrie & Simon: 3-4, 3-9, 3-24, 3-26, 3-27 (porphyrin has 26 \( \pi \) e-), 4-1, 4-10, 4-28

2. Show that \( \langle r \rangle = a/2 \mathbf{i} + b/2 \mathbf{j} + c/2 \mathbf{k} \) for three-dimensional particle in a box (i.e., the average position for a particle in a 3D box is in the center of the box)

3. For the following, I suggest using MathCad or Excel.
   a) Calculate energies of an electron in a 3-D box with \( a = 1 \) nm, \( b = 2 \) nm, and \( c = 20 \) nm for \( n_x = 1, 2, 3, n_y = 1, 2, 3, \) and \( n_z = 1, 2, 3 \). (Hint: There are 27 combinations of these quantum numbers.) Verify that there are no degenerate states.
   b) Predict which states would be degenerate if the box had dimensions \( a = 2 \) nm, \( b = 2 \) nm, and \( c = 20 \) nm. Repeat part (a) for a box of these dimensions.

You may find the following equations helpful (these are used in various places throughout the assignment).
\[
\int_0^1 x^m (1 - x)^n \, dx = \frac{m! n!}{(m + n + 1)!}
\]
\[
\int_0^a \sin^2 \left( \frac{n \pi x}{a} \right) \, dx = \frac{a}{2}
\]
\[
\int_0^a \sin \left( \frac{n \pi x}{a} \right) \cos \left( \frac{n \pi x}{a} \right) \, dx = 0
\]

Plus the ones in the back of the book!