CHE-372 Gustavus Adolphus College

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 π e-), 4-1, 4-10, 4-28

2. Show that $\langle \mathbf{r} \rangle = a/2\ \mathbf{i} + b/2\ \mathbf{j} + c/2\ \mathbf{k}$ 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).

$$\int_0^1 x^m (1-x)^n \, dx = \frac{m!n!}{(m+n+1)!}$$

$$\int_0^a \sin^2\left(\frac{n\pi x}{a}\right) dx = \frac{a}{2}$$

$$\int_0^a \sin\left(\frac{n_x \pi x}{a}\right) \cos\left(\frac{n_x \pi x}{a}\right) dx = 0$$

Plus the ones in the back of the book!