

Due March 14 at 3 pm

1. McQuarrie & Simon: 3-1b and 1c, 3-4, 3-9, 3-24, 3-26, 3-27 (porphyrin has $26 \pi e^-$)
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 $a = 1 \text{ nm}$, $b = 2 \text{ nm}$, and $c = 20 \text{ nm}$ 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 $a = 2 \text{ nm}$, $b = 2 \text{ nm}$, and $c = 20 \text{ nm}$. Repeat part (a) for a box of these dimensions.