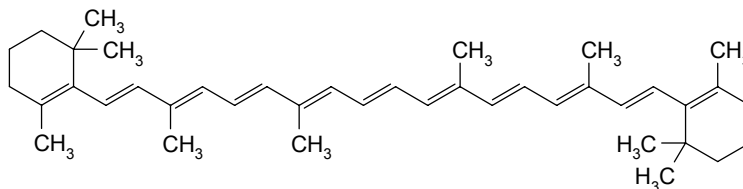# CHEM 260

Assignment 3

10. Use the "particle in a box" model to estimate the difference in energies of the HOMO and LUMO levels of β-carotene, and thence calculate the wavelength of the corresponding optical transition. * (Assume a box length equal to 21 bonds of 1.4 Å each. Calculate the energy levels and fill them, two at a time, with the 22 π electrons.)

11. The energy levels for a particle in a cubic box are given by

$$E = \left(n^2 + m^2 + k^2\right) E_{100} \qquad \text{where } E_{100} = \hbar^2/(8ma^2)$$

where n, m and k are quantum numbers. Using Excel (recommended) or otherwise, make a table with the following headings

n	m	k	degeneracy	E/E_{100}

showing all the energy levels up to, and including, $E = 19$ (in units of $E_{100} = h^2/8ma^2$).

> [**Note**: Don't bother to write out all degenerate states. For example, the three states (1,1,2), (1,2,1) and (2,1,1) are degenerate; just list one of them and put *3* in the degeneracy column.]

How many *levels* (distinct values of E) are there? How many *states*?

Suppose the energy levels are occupied by non-interacting particles which are allowed a maximum of two per state (like electrons in atomic or molecular orbitals). How many particles are needed to give a ground state system energy (total for all particles) of 354 (in our dimensionless units)? How many particles are needed to give a total energy of 388?

12. Write a short (maximum 1 page‡) essay# on one of the following topics:

    a) A summary of the need to invent quantum mechanics at the end of the nineteenth century. A suitable title might be "What a catastrophe!"

    b) A historical description of models for the structure of matter: "Earth, air, fire , water… and waves!".

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* This simple model does not quite work. Carrots are orange because they absorb blue light (450 nm).

‡ Using a word processor, one page at 1.5 line spacing gives about 30 lines, 300 words.

Yes, an essay, in proper English sentences (unlike this one).