Worksheet: Particle in a Box Wavefunctions I

Physical Chemistry I
Fall 2005
M. Francl

Using the skeleton notebook, PIBwavefns.nb, answer the questions below.

The general form for the particle in the box wavefunction is $\psi_n(x) = \left(\frac{2}{a}\right)^{1/2} \sin\frac{n\pi x}{a}$.

To warm up, calculate the probablity of finding the particle in the left-hand side of the box for n=1, 4 and a large n of your choosing. How do you define the "left-hand side"? How does the value change as n changes?

We noticed earlier that the probability of finding the particle became more spread out as n increased. We assessed this qualitatively by plotting the probability density for various n. A better measure of the spread of the particle is the uncertainty in the position. So, let's calculate the uncertainty in the position of the particle inside the box as n increases. The definition of the uncertainty is $\sigma_x^2 = \langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2$. Make a graph of the uncertainty versus n, choose any value you like for the length of the box. Sketch the graph below. Predict what will happen at very large n. Choose some very large n and see if your prediction is correct!

The molecule below is canthaxanthin, which is responsible for the characteristic pink color of flamingos. The source of the pigment is exogenous – in their natural habitat the birds consume shrimp which contain the pigment. Flamingos living in zoos need to be given a source of the protein or they will turn white! Let's make a model of the electron energies based on the free electron model (section 3-5 of Atkins) and predict the color of canthaxanthin. Take the C-C to be 154 pm, the C=C to be 135 pm, the C=O to be the mass of the electron to be 9.109×10^{-31} kg. Planck's constant is 6.626×10^{-34} J-sec.

What is the length of the box? How did you estimate it?

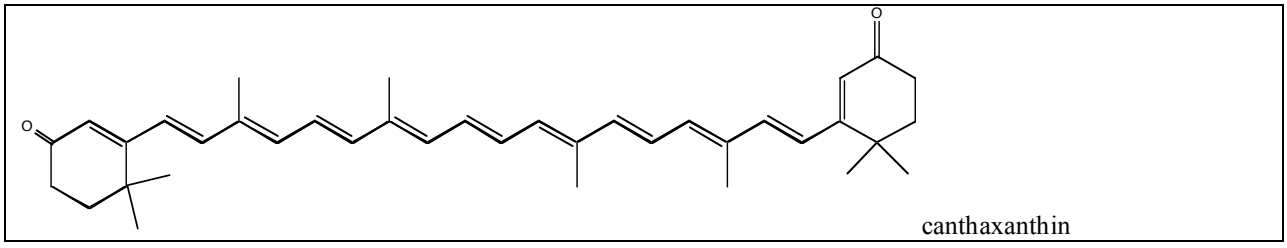
How many electrons are in the box?

What is the "HOMO"? the "LUMO"?

What is the change in energy for moving an electron from the HOMO to the LUMO?

What frequency corresponds to this? Is the frequency in the visible?

If the molecule absorbs at this frequency, what color is it?

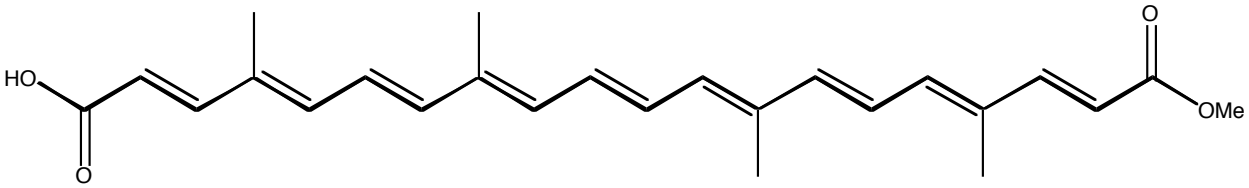


canthaxanthin

The Culture of Chemistry

What do flamingos, Cheez-Whiz and Quantum Chemistry have in common?

Carotenoid dyes, based on a linear conjugated diene skeleton, provide nature with some colorful accents. Canthaxanthin, for example, is fed to captive flamingos to produce their characteristic pink color (a similar pigment found in brine shrimp does the same favor for wild flamingos). Canaries, whose signature color is a greenish yellow, can be turned red if they are fed paprika during their molt. The new feathers will grow in orange-red. If you're tired of only changing the color of your hair, you can try for a pumpkin look for fall. The compound that gives this class of vegetable pigments its name — β-carotene — when consumed in large quantities by humans, will turn them orange. [Really, but don't try this at home! It was observed clinically in Britain during WW II when food shortages led some people to include large amounts of carrots in their diets.] And if you thought the bright color of Cheez-Whiz and Cheetos was artificial -- it's not. Bixin or annatto, a natural pigment used for centuries is the source of that unforgettable orange. Researchers have recently elucidated the biochemical pathway for the synthesis of bixin and are pursuing genetic engineering approaches to its bulk synthesis in tomatoes [Florence Bouvier in *Science*, 300:2089-2091, June 27, 2003].



Bixin