APh161: Physical Biology of the Cell
Homework 2
Due Date: Tuesday, February 3, 2009

"To do successful research, you don't need to know everything. You just need to know of one thing that isn't known." – A. L. Schawlow

Reading: Read chap. 14 of "Molecular Biology of the Cell" by Alberts *et al.* See the online version of the book posted on the website and read the section on "Chloroplasts and Photosynthesis". This will give you a better sense of the energetics of the photosynthetic process and on the management of charges (electron and proton transfer). Read chap. 6 of PBoC.

1. Photosynthesis: Your Turn.

(a) Write a two-paragraph description of the nature of photosynthesis that would be appropriate for readers of "Scientific American". Key points that you should touch upon include: relevance of photosynthesis to life on Earth and the mechanisms of photosynthesis. Your essay should be readable by an interested high-school student.

(b) Make a syllabus for 5 lectures on photosynthesis. Your syllabus should say what topics you will cover. Make sure that this includes some statement of what estimates you would do, what experiments you would describe and what calculations you would do. Try to view this with a fresh perspective and don't feel the need to do anything the same way that I did. This should be one paragraph or less. You are making a syllabus with bullets.

(c) Experiments and photosynthesis. Give a brief description (1-paragraph maximum) of three experiments that have shed light on the nature of photosynthesis. Make sure to say the concept of the experiment, how it was implemented and the nature of the resulting data.

NOTE: this problem will be graded by Rob.

2. Respiration and Photosynthesis: A Feeling for the Macroscopic Numbers.

Most of this problem was motivated by the outstanding book **Guesstimation** by Lawrence Weinstein and John Adam. I highly recommend this book to all of you and believe strongly that even if you think estimates of this kind are "trivial", they are well worth your time. Some of the most important and interesting episodes in the history of science having involved estimates. Two of the most important are: i) when Newton estimated the acceleration of the moon as it "falls" around the Earth and compared it to the acceleration at the Earth. He found that they differed by nearly a factor of 3600, corresponding to the 60-fold difference in distance from the center of the Earth, suggesting the inverse square law, ii) Kelvin's estimates of the age of the Earth and the lifetime of the sun. Both of Kelvin's estimate were inconsistent with geology and foreshadowed the discovery of radioactivity.

In problems like this, I want to see clear statements of your assumptions, the key orders of magnitude that dictate your estimates and some sort of summarizing statement about what the estimates mean. Further, these estimates should involve very little looking stuff up online.

(a) The Keeling curve shows two extremely interesting features of the overall CO_2 budget of the Earth. First, it is most famous for illustrating the impact of humanity on the atmospheric composition, revealed through the trend of increasing CO_2 over time. However, the second interesting feature of the Keeling curve is the annual variation in CO_2 concentrations which reflect the summer-winter cycle of the greener northern Hemisphere. Keeling's son Ralph has now made it his mission to make careful measurements of the time evolution of atmospheric oxygen.

Several interesting links on this stuff are:

http://www.scivee.tv/node/4611

http://explorations.ucsd.edu/Features/Keeling_Curve/

and the Scripps feature posted with this homework.

Spend a little time thinking about atmospheric oxygen by making a simple estimate of how long it would take for the breathing of humans to use up the atmospheric oxygen if photosynthetic organisms were not around to perform carbon fixation. There are a variety of different ways to approach this. First, in class I already worked out the number of molecules in the atmosphere (and its mass) so you could figure out how much O_2 there is that way. Alternatively, you could just try to figure out how long it would take for all humans to have breathed in the whole atmosphere and by thinking about what fraction of the O_2 is combusted. For the purposes of this estimate, just imagine that with each breath you are burning glucose (you might want to write down the relevant reaction). Figure out the mass per breath and use that to figure out the number of breaths in the atmosphere (given the atmospheric mass). Weinstein and Adam point out that we can use CPR and sustain someone in life, so we don't exhaust all of the oxygen with each breath. Again, you should not have to look up very much to solve this problem.

(b) Make an estimate of the amount of CO_2 absorbed per year by the growth of a new forest on one km^2 of land. Hint: figure out the number of trees in a 1 km^2 area and average over the time from when the trees are saplings to fully grown to figure out how much carbon was used to make the trees.

Though it is not critical to the estimate, you might enjoy taking a look at the Earth Observatory to get a sense of the leaf area index:

http://earthobservatory.nasa.gov/Observatory/Datasets/lai.modis.html.

A second way to do this problem that you should also try is to figure out the area per tree. Now, imagine that the roughly 1000 W/m^2 of power resulting from incident sunlight is used to fix carbon (with some efficiency depending both upon what fraction of the day the sunlight is present and the actual efficiency of light absorption and energy usage - use the geometric mean rule by trying to make an upper and lower bound on how efficient this can be). Then use the rule of thumb that ten photons are needed for each carbon fixed. NOTE: in the solutions, we will give you the best current estimates of this number resulting from measurements on tree plantations.

(c) There is much discussion about deforestation and its impact on the environment. Make an estimate of the total CO_2 released into the atmosphere as a result of burning of forests for as long as man has used fire. Work out this number in parts per million for atmospheric CO_2 and compare this to the numbers you see in the Keeling curve. In addition, make a simple estimate of the total energy released by such burning.

3. Molecular Orbitals and the HOMO-LUMO Gap.

In this problem, you will work out for yourselves many of the ideas discussed in class using the case study of the H_2 molecule, but now generalized to other geometries. Recall that the main point of this part of the course was to develop some understanding of the electronic structure of molecules and how it dictates the light absorption by those molecules. In particular, I was trying to give you a flavor for how "Huckel theory" works - this is really a highly-simplified scheme for working out the electronic structure for molecular orbitals involving the p_z orbitals on the atoms. More generally, to quote an important figure in the development of our modern thinking on chemical bonds, "The role of quantum chemistry is to understand the elementary concepts of chemistry and to show what are the essential features of chemical behavior" (from Jeremy Burdett in his "Chemical Bonds"). Follow the scheme described in class by calling off-diagonal elements of the Hamiltonian matrix $\beta = \langle i|H|j\rangle$, where $i \neq j$ and $\alpha = \langle i|H|i\rangle$. Further, only consider near-neighbor interactions (i.e. we will ignore any possible overlap integrals between atoms that are not exactly adjacent.)

(a) Using the method of derivation performed in class for the two-atom molecule, work out the Hamiltonian matrix, find the energy eigenvalues and the wave functions (in terms of α and β) for a molecule with three atoms at the vertices of an equilateral triangle. Make an energy level diagram that shows the eigenvalues and show how the electron states are filled. Assume that each atom contributes one electron.

(b) Consider a four-atom square molecule (a toy model of cyclobutadiene, C_4H_4). Using an analogy to what you did in the previous part of the problem, but without all of the detailed derivations, write the Hamiltonian matrix. With this Hamiltonian matrix, find the eigenvalues and wave functions and compute the HOMO-LUMO gap in terms of the parameters α and β. Assume that there is no coupling between orbitals across the diagonals of the square. Further, make an energy level diagram and show the electron occupancies of each state. Finally, compute the wavelength of absorption for this molecule using the simple ideas we have worked out in class, and letting $\alpha = 0$ and $\beta = -2.4$ eV (see Melvin Hanna, "Quantum Mechanics in Chemistry", pg. 206).

I have tried to hunt around for some places where you can learn a little more about the parameters that show up in these kinds of models. One site that emphasizes the application to solids is:

http://www.icmm.csic.es/jcerda/EHT_TB/TB/Periodic_Table.html

4. Free Electron Model of Pigment Electronic Structure.

In class I quickly worked out a toy model of the electronic structure of linear chain molecules. In this problem, your job is to write up a clear, pedagogical derivation of that problem culminating in two plots: 1) a plot of the HOMO-LUMO gap as a function of the length of the linear chain molecule and 2) a plot of the absorption wavelength as a function of the length of the linear chain molecule.

5. A Feeling for the Numbers: Microbes as the Unseen Majority

One of the key arguments that I will make throughout the course is that sometimes just having a feel for magnitudes is a useful guide to intuition. Indeed, our model building will usually follow the sequence: simple estimates and feeling for the numbers, simple toy models, more realistic models. For this problem, use the article you read last week entitled "Prokaryotes: The Unseen Majority" as the basis for your estimates.

(a) We will think of *E. coli* as our biological standard ruler. This cell has hall of fame status in biology and it is important that you have a sense of what these cells are like. Justify the assumption that a typical (i.e. *E. coli*) bacterial cell has a volume of 1 μm^3. Also, express this volume in femtoliters.

The claim is made (in "Prokaryotes: the Unseen Majority") that in the top 200 m of the world's oceans, there are roughly 10^{28} prokaryotes. Work out the total volume taken up by these cells in m^3 and km^3. Compare that to the total volume taken up by humans on Earth.

(b) Also, recall that roughly 2-3 kg of bacteria are to be found in the waste factory of your large intestine. Make an estimate of the total number of bacteria inhabiting your intestine and then all of the intestines of all of the humans currently on the Earth. Compare this to the number of cells in your body which you can estimate by noting the typical sizes of eukaryotic cells. Make sure to explain the entirety of your rationale for these estimates.

(c) If a particular protein in an *E. coli* cell is found there at nM concentrations, how many molecules are there per cell? Are you happy with the notion of a "concentration" in this case? Explain your reasoning. Make a plot of the number of copies of a molecule in an *E. coli* cell as a function of the concentration - make the plot for concentrations from nM to mM.

(d) Bacteriophage are the viruses that infect bacteria. Given that the concentration of phage is tenfold or more higher than that of bacteria, report the concentration of phage in the ocean in mg/mL. Then, use this to make an estimate of the total number of phage on the Earth. This number will come in handy in our initial estimates about evolution.