

1.5 Franklin's estimate

The estimate of Avogadro's number in Section 1.5.1 came out too small partly because we used the molar mass of water, not of oil. We can look up the molar mass and mass density of some sort of oil available in the eighteenth century in the *Handbook of chemistry and physics* (Lide, 2006). The *Handbook* tells us that the principal component of olive oil is oleic acid and gives the molar mass of oleic acid (also known as 9-octadecenoic acid or $\text{CH}_3(\text{CH}_2)_7\text{CH}=\text{CH}(\text{CH}_2)_7\text{COOH}$) as 282 g mole^{-1} . We'll see in Chapter 2 that oils and other fats are triglycerides, made up of three fatty acid chains, so we estimate the molar mass of olive oil as a bit more than three times the value for oleic acid. The *Handbook* also gives the density of olive oil as 0.9 g cm^{-3} .

Make an improved estimate of N_{mole} from these facts and Franklin's original observation.

1.6 Atomic sizes, again

In 1858, J. Waterston found a clever way to estimate molecular sizes from macroscopic properties of a liquid, by comparing its surface tension and heat of vaporization.

The surface tension of water, Σ , is the work per unit area needed to create more free surface. To define it, imagine breaking a brick in half. The two pieces have two new surfaces. Let Σ be the work needed to create these new surfaces, divided by their total area. The analogous quantity for liquid water is the surface tension.

The **heat of vaporization** of water, Q_{vap} , is the energy per unit volume we must add to liquid water (just below its boiling point) to convert it completely to steam (just above its boiling point). That is, the heat of vaporization is the energy needed to separate every molecule from every other one.

Picture a liquid as a cubic array with N molecules per centimeter in each of three directions. Each molecule has weak attractive forces to its six nearest neighbors. Suppose it takes energy ϵ to break one of these bonds. Then the complete vaporization of 1 cm^3 of liquid requires that we break all the bonds. The corresponding energy cost is $Q_{\text{vap}} \times (1 \text{ cm}^3)$.

Next consider a molecule on the *surface* of the fluid. It has only five bonds—the nearest neighbor on the top is missing (suppose this is a fluid–vacuum interface). Draw a picture to help you visualize this situation. Thus, to create more surface area requires that we break some bonds. The energy needed to do that, divided by the new area created, is Σ .

- For water, $Q_{\text{vap}} = 2.3 \cdot 10^9 \text{ J m}^{-3}$ and $\Sigma = 0.072 \text{ J m}^{-2}$. Estimate N .
- Assuming the molecules are closely packed, estimate the approximate molecule diameter.
- What estimate for Avogadro's number do you get?

1.7 Tour de France

A bicycle rider in the Tour de France eats a lot. If his total daily food intake were burned, it would liberate about 8000 kcal of heat. Over the three or four weeks of the race, his weight change is negligible, less than 1%. Thus, his energy input and output must balance.

Let's first look at the mechanical work done by the racer. A bicycle is incredibly efficient. The energy lost to internal friction, even including the tires, is negligible. The expenditure against air drag is, however, significant, amounting to 10 MJ per day. Each day, the rider races for 6 hours.

- Compare the 8000 kcal input to the 10 MJ of work done. Something's missing! Could the missing energy be accounted for by the altitude change in a hard day's racing?

Regardless of how you answered (a), next suppose that on one particular day of racing there's no net altitude change, so that we must look elsewhere to see where the missing energy went. We have so far neglected another part of the energy equation: the rider gives off *heat*. Some of this is radiated. Some goes to warm up the air he breathes in. But by far the greatest share goes somewhere else.

The rider *drinks a lot of water*. He doesn't need this water for his metabolism—he is actually creating water when he burns food. Instead, nearly all that liquid water leaves his body as water *vapor*. The thermal energy needed to vaporize water appeared in Problem 1.6.

- b. How much water would the rider have to drink for the energy budget to balance? Is this reasonable?

Next let's go back to the 10 MJ of mechanical work done by the rider each day.

- c. The wind drag for a situation like this is a backward force of magnitude $f = Bv^2$, where B is some constant. We measure B in a wind-tunnel to be 1.5 kg m^{-1} . If we simplify by supposing a day's racing to be at constant speed, what is that speed? Is your answer reasonable?

PROBLEMS

2.1 *All Greek to me*

Now's the time to learn the Greek alphabet. Here are the letters most often used by scientists. The following list gives both lowercase and uppercase (but omits the uppercase when it looks just like a Roman letter):

$\alpha, \beta, \gamma/\Gamma, \delta/\Delta, \epsilon, \zeta, \eta, \theta/\Theta, \kappa, \lambda/\Lambda, \mu, \nu, \xi/\Xi, \pi/\Pi,$
 $\rho, \sigma/\Sigma, \tau, \upsilon/\Upsilon, \phi/\Phi, \chi, \psi/\Psi, \omega/\Omega$

When reading aloud we call them alpha, beta, gamma, delta, epsilon, zeta, eta, theta, kappa, lambda, mu, nu, xi (pronounced "ksee"), pi, rho, sigma, tau, upsilon, phi, chi (pronounced "ky"), psi, omega. Don't call them all "squiggle."

Practice by examining the quote given in Chapter 1 from D'Arcy Thompson, which in its entirety reads: "Cell and tissue, shell and bone, leaf and flower, are so many portions of matter, and it is in obedience to the laws of physics that their particles have been moved, moulded, and conformed. They are no exception to the rule that $\Theta\epsilon\delta\sigma\ \alpha\epsilon\iota\ \gamma\epsilon\omega\mu\epsilon\tau\rho\epsilon\iota$." From the sounds made by each letter, can you guess what Thompson was trying to say? [Hint: ζ is an alternate form of σ .]

2.2 *Do-it-yourself proteins*

This book contains some molecular structure pictures; you can easily make many more yourself. Download RasMol from <http://www.umass.edu/microbio/rasmol/index.html> (or <http://openrasmol.org>), or get some other free molecular viewing application.⁹ Now go to the Protein Data Bank,¹⁰ <http://www.rcsb.org/pdb/>. On the main page, try searching for and viewing molecules (see also the "molecule of the month" department, from which the examples below were taken). Once you get the molecule's main entry, click "explore" on the right, then "view" and download in RasMol format. Play with the many RasMol options. Alternatively, you can just click quickpdb for a viewer that requires no separate application. Here are some examples; several are discussed in this and later chapters:

- a. thrombin, a blood-clotting protein (code 1ppb).
- b. insulin, a hormone (code 4ins).
- c. myosin, a molecular motor (code 1b7t).
- d. the actin-myosin complex (code 1alm). This entry shows a model of one myosin motor bound to a short actin filament formed of five molecules, based on data from electron microscopy. The file contains only alpha carbon positions for the proteins, so you'll need to use backbone diagrams when you look at it.
- e. rhinovirus, responsible for the common cold (code 4rhv).

⁹Protein Explorer, also available at <http://www.umass.edu/microbio/rasmol/index.html> requires installation of additional software. Other popular packages include PyMol (<http://pymol.sourceforge.net>) and VMD (<http://www.ks.uiuc.edu/Research/vmd/>).

¹⁰The PDB is operated by the Research Collaboratory for Structural Bioinformatics (RCSB). You can also find RasMol there under "software."

- f. myoglobin, an oxygen-storing molecule found in muscles (code 1mbn). Myoglobin was the first protein structure ever determined.
- g. DNA polymerase (code 1tau).
- h. the nucleosome (code 1aoi).

Use your mouse to rotate the pictures. Use the measurement feature of RasMol to find the physical size of each object. Selectively color only the hydrophobic residues. Try the “stereo” option. Print the ones you like.

2.3 *Do-it-yourself nucleic acids*

Go to the Nucleic Acid Database, <http://ndbserver.rutgers.edu/>. Download coordinates and view, using RasMol or another software:

- a. the B-form of DNA (code bd0001). Choose the space-filling representation and rotate the molecule to see its helical structure.
- b. transfer RNA (code trna12).
- c. RNA hammerhead enzyme, a ribozyme (code urx067).
- d. the complex of integration host factor bound to DNA (code pdt040). Try the cartoon display option.

2.4 *Do-it-yourself small molecules*

Go to <http://molbio.info.nih.gov/cgi-bin/pdb> and search for some small molecule mentioned in this chapter. You'll probably find PDB files for larger molecules binding the one you chose. Look around.

2.5 *Do-it-yourself micelles and bilayers*

Go to <http://moose.bio.ucalgary.ca/>, <http://persweb.wabash.edu/facstaff/fellers/>, <http://www.umass.edu/microbio/rasmol/bilayers.htm>, or some other database with lipid structures.

- a. Go to “downloads” at the first site mentioned and look at the file m65.pdb, which shows a micelle containing 65 molecules of the surfactant. This picture is the output of a molecular simulation. Tell RasMol to remove the thousands of water molecules surrounding the micelle (uncheck “hydrogen” and “hetero atoms”), so you can see it.
- b. At the second site mentioned, get the coordinates of the dipalmitoyl phosphatidylcholine bilayer and view it. Again remove the surrounding water. Rotate it to see the layer structure.