

Problem set 1

(Discussion on April 22, 2021)

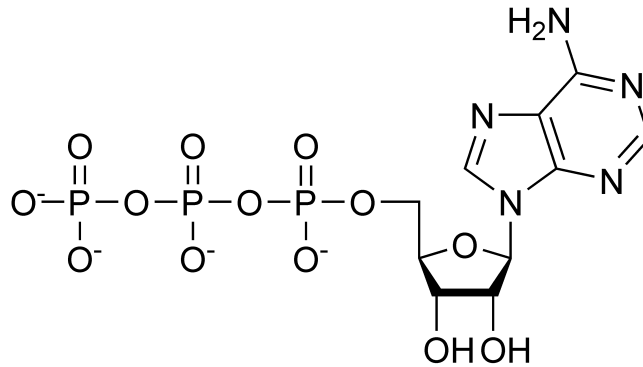
Problem 1

Quantifying *E. coli*. One of the most common model organisms for research and a key player in biotechnology is *Escherichia coli*, a simple rod-shaped bacterium. In the following, you can approximate *E. coli* cells as cylinders with $1\ \mu\text{m}$ diameter and $2\ \mu\text{m}$ length. You can round to the nearest order of magnitude.

- What is the volume (in μm^3 and L) of an *E. coli* cell?
- How many molecules of a certain kind are in one *E. coli* cell, if their concentration is 1 nM, 1 mM, 1 M?
- If we assume that molecules are very approximately on a cubic lattice, what is the spacing between molecules at 1 nM? 1 mM? 1 M?
- What is the mass of an *E. coli* cell, if we assume that it roughly has the same density as water?
- Does *E. coli* really have the same mass as water (google it!)? What are important consequences of the difference?
- Swimming *E. coli* swim with $\approx 30\ \mu\text{m}/\text{s}$. How many body lengths/s does this correspond to? How does this compare to a top-level human swimmer? To a great white shark (which swim with 30 miles/h)?

Problem 2

ATP hydrolysis. Adenosine triphosphate (or ATP for short) is the “energy currency” of the cell. The energy is stored in the spatial arrangement of three negatively charged phosphate groups, see figure. The energy is released when the last phosphate group (also called the γ -phosphate) is broken off or released, i.e. when ATP is *hydrolyzed* to ADP (adenosine diphosphate). You can compute a simple estimate of the energy released upon ATP hydrolysis by considering the electrostatic energy of the phosphate groups. You can treat the phosphate groups as point charges on a line, with the γ -phosphate having a charge of $-2e$ and the other two each with a charge of $-1e$, separated by a distance of 0.3 nm between phosphate groups, and use Coulomb’s law to compute the potential energy.



- What is the energy difference between ATP and ADP, if you assume that the released phosphate moves infinitely far away and that the reaction takes place in vacuum?
- How does the results from the previous question change, if the reaction takes place in water?

Problem 3

Van der Waals interactions. The (non-electrostatic and non-covalent) interactions between atoms are often modeled with a so-called Lennard-Jones or “12-6” potential. The energy as a function of the distance between the atoms r is given by the functional form:

$$E(r) = 4\epsilon \left(\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right) \quad (1)$$

- For what distance is the interaction energy minimal? What is the energy at the minimum?
- Draw (by hand or, better, by using a software of your choice) the potential for parameters $\epsilon = 1.66 \cdot 10^{-21}$ J and $\sigma = 3.4 \cdot 10^{-10}$ m.
- Can you think of a molecular interpretation of the two terms in the energy function?