5.111 Principles of Chemical Science
Fall 2008

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Solutions to selected biology-related questions from problem sets for lectures 1-9

<u>Review of fundamentals</u>

A.
Lisinopril, sold under the brand names of Prinivil® (Merck) or Zestril® (AstraZeneca), is a small molecule drug used to treat high blood pressure and heart failure. It works by inhibiting the production of angiotensin, a signaling molecule found in the blood that causes vasoconstriction (narrowing of blood vessels) and increased blood pressure. Lisinopril has a mass percentage composition of 62.2% carbon, 7.7% hydrogen, and 10.4% nitrogen, with the balance being oxygen. What is the empirical formula of lisinopril?

Molecular weight of $C_6H_{12}O_6$ = 180.16

$$400.\ \text{g } C_6H_{12}O_6 \times \frac{1\ \text{mol}}{180.16\ \text{g } C_6H_{12}O_6} = 2.2\underline{2}0\ \text{mol of } C_6H_{12}O_6$$

$$2.2\underline{2}0\ \text{mol of } C_6H_{12}O_6 \times \frac{6\ \text{mol } O_2}{1\ \text{mol } C_6H_{12}O_6} = 13.\underline{3}2\ \text{mol } O_2$$

$$13.\underline{3}2\ \text{mol } O_2 \times (32.00\ \text{g / mol}) = 42\underline{6}.2\ \text{g}$$

amount of O in Lisinopril = 100.0 g – 62.2 g – 7.7 g – 10.4 g
= 19.7 g of O

We can now fill in the table to calculate the molar ratios:

element	**amt. in 100 g lisinopril**	**# of moles**	**molar ratios** (x 3)
C	62.2 g	62.2 g/(12.01 g•mol^{-1}) = 5.1$\underline{7}$9 mol	6.9$\underline{7}$7 (20.$\underline{9}$3)
H	7.7 g	7.7 g/(1.0079 g•mol^{-1}) = 7.64 mol	10.3 (30.9)
N	10.4 g	10.4 g/(14.01 g•mol^{-1}) = 0.74$\underline{2}$3 mol	1.0$\underline{0}$0 (3.0$\underline{0}$0)
O	19.7 g	19.7 g/(16.00 g•mol^{-1}) = 1.2$\underline{3}$1 mol	1.6$\underline{5}$8 (4.9$\underline{7}$4)

$$\mathbf{C_{21}H_{31}N_3O_5}$$

B.
Through a process called cellular respiration (or oxidative metabolism), your body converts energy stored in the molecular bonds of sugars (such as glucose) into a form of energy that can be used directly by your cells. The reaction for the oxidative metabolism of glucose is

$$C_6H_{12}O_6 + 6O_2 \Rightarrow 6CO_2 + 6H_2O\ (+\ \text{energy}).$$

In order for your body to oxidize 350. g of glucose, what mass of molecular oxygen (O_2) is required in the reaction?

$C_6H_{12}O_6 + 6\ O_2 \rightarrow 6\ CO_2 + 6\ H_2O$

First, convert grams of $C_6H_{12}O_6$ (glucose) to moles of glucose.
MW of $C_6H_{12}O_6$ = 180.16 g/mol

$$350.\text{ g} \times \frac{\text{mol}}{180.16\text{ g}} = 1.9\underline{4}3 \text{ mol of glucose}$$

1 mole of glucose reacts with 6 moles of O_2. We can now convert moles of glucose to grams of O_2 using this 1:6 ratio and the mw of O_2. MW of O_2 = 32.00 g/mol.

$$1.9\underline{4}3 \text{ mol glucose} \times \frac{6 \text{ mol } O_2}{1 \text{ mol glucose}} \times \frac{32.00 \text{ g } O_2}{\text{mol } O_2} = 37\underline{3}.056 \text{ g } O_2$$

373 g O_2

The Quantum World

C.

Research in the Bawendi lab at MIT focuses on the synthesis and application of quantum dots, fluorescent semiconductor crystals. The green quantum dot depicted in the lecture #3 notes emits photons with a wavelength of 535 nm. Calculate the frequency of the photons emitted.

$\lambda\nu = c$
$\nu = c/\lambda$
$\nu = (2.998 \times 10^8 \text{ m}\bullet\text{s}^{-1})/(535 \times 10^{-9} \text{ m})$
$\nu = 5.60 \times 10^{14} \text{ s}^{-1}$

D.

Carotenoids are a class of molecules found in organisms that undergo photosynthesis. These organic molecules facilitate increased energy production by enabling absorption of blue light. Calculate the energy in 1 mole of 455 nm (blue) light.

$$E = hc/\lambda = \frac{(6.626 \times 10^{-34} \text{ J}\bullet\text{s})(2.998 \times 10^8 \text{ m}\bullet\text{s}^{-1})}{455 \times 10^{-9} \text{ m}}$$

$E_i = 4.3\underline{6}6 \times 10^{-19}$ J (This is the energy *per photon*)

$$\frac{4.366 \times 10^{-19} \text{ J}}{\text{(photon)}} \times \frac{6.022 \times 10^{23} \text{ (photons)}}{\text{mol}} = \mathbf{2.63 \times 10^5\ J} \text{ of energy in 1 mol}$$

E.

Fluorescent molecules (known as fluorophores) are widely used by chemists and biologists to study sub-cellular molecules, including proteins, DNA, and RNA. In the most straightforward applications, fluorophores are appended to a bio-molecule of *interest and used to image the bio-molecule's cellular location. The fluorescence imaging process involves the excitation of a fluorophore with a photon of energy, resulting in a brief (1-10 ns) excited state that is followed by the release of a photon with a second, lower energy.*

Imagine that you are studying a protein involved in tumor metastasis (spreading). Based on previous studies, you hypothesize that the protein localizes to the nucleus in tumor cells. To determine the sub-cellular location of your protein, you label it with a fluorophore that can be excited by light in the range of 620. to 674 nm.

The lab's fluorescent microscope is currently set up with a He-Ne laser for excitation. The laser produces a beam of light with a per-photon energy of 3.14 x 10^{-19} J and an intensity of 13 W (J/s).

(a) Calculate the wavelength of the light emitted by the He-Ne laser.
(b) Does the He-Ne laser beam have an appropriate energy to excite your fluorophore (does it fall within the excitation range)?
(c) Calculate the number of photons emitted by the laser per second.

(a) We know the energy of the laser = 3.14 x 10^{-19} J.

$$E_{photon} = h\nu = hc/\lambda$$

$$\lambda = hc/E_{photon}$$

$$\lambda = \frac{(6.626 \times 10^{-34}\ \text{J}\bullet\text{s})\ (3.00 \times 10^{8}\ \text{ms}^{-1})}{3.1\underline{4} \times 10^{-19}\ \text{J}} = 6.3\underline{3}1 \times 10^{-7}\ \text{m}$$

λ = **633 nm**

(b) Yes. The wavelength (633 nm) falls within the excitation range of 620 to 674 nm

(c) I = 13 W or 13 J/s

$$\frac{13\ \text{J}}{\text{s}} \times \frac{\text{photon}}{3.14 \times 10^{-19}\ \text{J}} = 4.\underline{1}4 \times 10^{19}\ \text{photons/s}$$

4.1 x 10^{19} photons

F.

Proton therapy is a form of radiation therapy used to shrink tumors by aiming high-energy protons (H^+ atoms) at cancerous cells and thereby damaging DNA and promoting cell death. The large relative mass of hydrogen ions in comparison to x-rays results in minimal scattering in the tissue, meaning less damage to healthy tissue surrounding a target tumor. If a proton accelerator produces a beam of protons (mw = 1.008 g/mol) with an average speed of 2.11 x 10^7 m/s, what is the wavelength of the protons?

We can use the DeBroglie equation for the calculation of the wavelength, but first we need to calculate the mass of the H^+ ion in kg:

$$\text{mass of one hydrogen ion} = \frac{1.008 \times 10^{-3}\ \text{kg/mol}}{6.0221 \times 10^{23}\ \text{mol}^{-1}} = 1.67\underline{3}8 \times 10^{-27}\ \text{kg}$$

We can now calculate the DeBroglie wavelength:

$$\lambda = h/p = h/(mv) = \frac{6.626 \times 10^{-34}\ \text{kg}\bullet\text{m}^2\bullet\text{s}^{-1}}{(1.67\underline{3}8 \times 10^{-27}\ \text{kg})(2.11 \times 10^{7}\ \text{m/s})}$$

$\boldsymbol{\lambda = 1.88 \times 10^{-14}}$ **m**