NAME

SIS (FERPA) ID (not JHED ID)

AS.250.315 Problem set 1

As in the dry run: write your name and SIS ID in their respective locations: 2" from the top margin and 1.5" (Name) and 5" (SIS ID) from the left margin). Write clearly which question you are answering (e.g., Problem 1) and keep to the positioning given on the pdf.

I agree to complete this homework without unauthorized assistance from any person or virtual person or pay-for-hire person.

Signature and Date

My collaborators on this homework are

For instructors only

Problem	max	earned
1	5	
2	10	
3	10	
4	5	
5	10	
6	10	
7	5	
8	20	
9	5	
10	10	
11	10	
total	100	

Problem 1

Assume that a reaction is exothermic and has a negative standard entropy under standard conditions and 298 K ($\Delta S^{\ominus} < 0$). Provide a criterion for spontaneity.

Problem 2

Assume that entropy and enthalpy changes are independent of temperature. A system in state A has an enthalpy of $-22\,\mathrm{kJ}$ and an entropy of $+7\,\mathrm{kJ\,K^{-1}}$. In state B, it has an enthalpy of $-12\,\mathrm{kJ}$ and an entropy of $+15\,\mathrm{kJ\,K^{-1}}$. At what temperatures will state B be favored?

Problem 3

Exhalation during breathing requires work because gas must be pushed out from the lungs against atmospheric pressure. Consider the work of exhaling $0.50\,\mathrm{dm^3}$ of vitiated air ($0.50\,\mathrm{dm^3}$ is a typical volume for a healthy adult) through a tube at the bottom of a cylinder equipped with a freely moving piston. The effort is against an atmospheric pressure P_{ex} of $1.00\,\mathrm{atm}$ ($101\,\mathrm{kPa}$). The exhaled air lifts the piston so that the change in volume is $\Delta V = 5.0 \times 10^{-4}\,\mathrm{m^3}$.

1. Calculate the work of exhaling.

2. Say that your real text book weighs approximately $1\,\mathrm{kg}$. How many books could the same amount of work lift from the floor to a shelf located at $1\,\mathrm{m}$ above the floor?

Problem 4

A typical 18- to 20-year-old man requires a daily energy input of about 12 MJ (1 MJ = 10^6 J) or about 2870 Cal; a woman of the same age needs about 9 MJ or about 2150 Cal. If the entire consumption were in the form of glucose, which has a specific enthalpy of 16 kJ g^{-1}, how much glucose should be consumed by the man and the woman to meet their energy needs?

Problem 5

The energy released at constant volume as heat by the combustion of the amino acid glycine (NH_2CH_2COOH) is -969.6 kJ mol^{-1} at 298.15 K. What is the standard enthalpy of combustion of glycine?

Problem 6

A chemist wants to develop a fuel by converting water back to elemental hydrogen and oxygen using coupled ATP hydrolysis to drive the reaction. Given that the standard Gibbs energy of formation for water is $-237\,\mathrm{kJ\,mol^{-1}}$ and that one mole of ATP hydrolyzed to ADP yields $-30\,\mathrm{kJ\,mol^{-1}}$, how much ATP is needed to yield one mole of H_2 gas?

Problem 7

Brown adipose cells play an important role in thermogenesis by burning lipids inefficiently, such that minimal work is done. The most common storage fatty acid in humans is palmitic acid (standard enthalpy of combustion at 298 K, $\Delta H_c^{\ominus}$, equal to $-9980\,\mathrm{kJ\,mol^{-1}}$). How many molecules of palmitic acid must be metabolized to raise the temperature of a 60 kg, hypothermic patient (34°C) back to physiological temperature (37°C)? Use the formula $q = m\,C\Delta T$, where C, the heat capacity of the body is approximately $3.6\,\mathrm{kJ\,kg^{-1}\,{}^{\circ}C^{-1}}$, and assume that all energy is released as heat.

Problem 8

Let's explore the hydrophobic effect.

1. Given a spherical particle of radius r, how does the surface area per particle (SA/particle) differ between a single particle and a spherical aggregate of 1,000 particles? Assume that the volume of the particles is perfectly combined to form the aggregate. (Or consider hexagonal closed packing if you recall the packing efficiency of identical spheres.)

2. Given your answer for part 1, explain which factor (entropy or enthalpy) drives aggregation and why.

3. For a system with only particles (such as proteins) and solvent molecules, the possible interactions are solvent−solvent, particle−particle and particle−solvent. Which of these interactions contributes most to aggregation and which contributes most to solvation? Explain.

4. Salting in is an effect by which the addition of some ions to a solution increases the solubility of dissolved particles, usually proteins. The exterior of proteins typically has ionizable groups that may interact electrostatically to form salt bridges. How does the addition of ions lead to an increase in solubility or a decrease in protein aggregates? Is this an entropic or enthalpic effect?

5. Salting out is an effect by which the addition of a high concentration of ions (much higher than the concentrations used for salting in) decreases the solubility of dissolved particles, causing the formation of aggregates. Explain how you think this effect occurs. It may help to think about what happens to ions when they enter a solution, and that there is a finite number of water molecules in a given volume of solution.

6. Given your answer for part 5 above, which interaction − ion−solvent or protein−solvent − is more favorable? Explain.

Problem 9

You have 1 L of a 2 M solution of imidazole. Imidazole is a weak base whose conjugate acid has a pK_a of 7.1. The initial pH is 10.5. What volume of concentrated HCl (12 M) do you need to add to drop the pH to 8.0? Are you surprised by your answer? Why or why not?

Problem 10

The pK_a of the R group of amino acids in folded proteins varies greatly because of their environments, which may stabilize or de-stabilize the conjugate base or acid. Rank the pK_a of the side chain carboxylic acid of glutamic acid in the following environments and explain your reasoning for each briefly.

a. In the protein exterior, adjacent to polar, non-ionizable residues
b. In the protein exterior, adjacent to a lysine
c. In the protein exterior, adjacent to another glutamic acid
d. In the protein interior (hydrophobic), adjacent to a methionine's sulfur position

Ranking:

Explanations:

a. In the protein exterior, adjacent to polar, non-ionizable residues

b. In the protein exterior, adjacent to a lysine

c. In the protein exterior, adjacent to another glutamic acid

d. In the protein interior (hydrophobic), adjacent to a methionine's sulfur position

Problem 11

Suppose you need to make a phosphate buffer at pH 7.5. In your lab, you have sodium phosphate monobasic (NaH_2PO_4, MW = $119.98\,\mathrm{g\,mol^{-1}}$) and sodium phosphate dibasic (Na_2HPO_4, MW = $141.96\,\mathrm{g\,mol^{-1}}$). How many grams of each solid will you weigh out to make 1 L of 50 mM phosphate buffer at pH 7.5? Use the phosphate pK_a values listed in your textbook.