Objective 12. Predict whether a reaction occurs using thermodynamics.

Key ideas: Does a reaction occur? Some reactions occur spontaneously; others do not.

 ΔG is the criterion used to predict whether a reaction occurs spontaneously: $\Delta G < 0$ means spontaneous reaction.

Two driving forces determine whether a reaction occurs spontaneously: enthalpy and entropy.

 $\Delta G = \Delta H - T\Delta S$. Compare ΔH and ΔS . Determine T at which reaction occurs or not.

Back to equilibrium. $K_{eq} > 1$ means more products than reactants. $\Delta G < 0$ means spontaneous. So ΔG is related to Keq: $\Delta G = -RT \ln K_{eq}$ where R = gas constant = 8.31 J/mole K and T = temperature in K.

Practice problems solutions:

There are two driving forces for a reaction: enthalpy and entropy. These two thermodynamic quantities are related by the equation:

$$\Delta G = \Delta H - T \Delta S$$

(1)

where ΔG is the change in free energy, ΔH is the change in enthalpy, and ΔS is the change in entropy. Free energy is the energy that is freely available in a system to do work. For a physical process or chemical reaction, a net decrease in free energy, i.e., $\Delta G < 0$, means that the process or reaction occurs spontaneously. For a reaction to occur spontaneously, $\Delta G < 0$. See Equation (1).

(i) If $\Delta H > 0$, does it help ΔG be less than 0? Answer: NO. If If so, ΔH is positive (right side of equation), it helps ΔG be positive. If $\Delta H < 0$, the reaction is favored by enthalpy.

(ii) If $\Delta S > 0$, does it help ΔG be less than 0? Answer: YES. If If so, ΔS is positive, then -T ΔS is negative (right side of equation), it helps ΔG be negative. If $\Delta S > 0$, the reaction is favored by entropy.

The sign and magnitude of ΔH and ΔS determines the sign of ΔG .

1. Predict the sign (> 0, = 0, or < 0; K is > 1 or < 1) of the specified quantities for the following processes. You will be able to predict the sign without doing a calculation for some reactions and quantities. Use a Table of thermodynamic values as needed. Give reasons for your answer.

	q	work	ΔH	ΔS	ΔG	К
Combustion of propane (used in bbq grills)						
CO_2 (s)> CO_2 (g) (sublmation of dry ice)						

Answers:

Propane combustion reaction: $C_3H_8(g) + 5 O_2(g) --> 3 CO_2(g) + 4 H_2O(g)$

	q	work	ΔH	ΔS	ΔG	К
Combustion of propane (used in bbq grills)	< 0 rxn is exothermic	< 0 ∆n>0, ∆V>0 so w<0	< 0 rxn is exothermic	> 0 more moles of products than reactants	< 0 rxn occurs spontaneously	> 1 rxn occurs spontaneously
CO ₂ (s)> CO ₂ (g) (sublmation of dry ice)	> 0 rxn is exothermic	< 0 Δn>0, ΔV>0 so w<0	> 0 rxn is exothermic	> 0 gas has higher entropy than solid	< 0 rxn occurs spontaneously	> 1 rxn occurs spontaneously

2. You know salt, NaCl, dissolves in water. But limestone (calcium carbonate, CaCO₃) does not dissolve in water.

a. Write a chemical equation that represents the dissolution of each solid in water. (Hint: solid ---> aqueous ions) b. Determine whether each reaction is exothermic or endothermic. What experimental observation tells you that this reaction is exothermic? Use Hess' law to calculate c to confirm your answer. Is this reaction favored by enthalpy? (Answer: Δ H is approximately 4 kJ/mole for NaCl and between -10 and -15 kJ/mole for CaCO₃)

c. Determine ΔS for this reaction. Is this reaction favored by entropy? (Answer: ΔS is approximately 40 J/K mole for NaCl and between -200 and -210 J/K mole for CaCO₃)

d. Calculate ΔG at 25°C. Does this calculation show NaCl is soluble in water? Does this calculation show CaCO₃ is not soluble in water?

e. There is a temperature at which NaCl (s) does not dissolve in water. ΔH and ΔS does not change with temperature but ΔG does. Use $\Delta G = \Delta H - T\Delta S$. Set $\Delta G = 0$ and substitute the numerical value for ΔH and ΔS into this equation and solve for T. Is it possible for NaCl not to dissolve at this T?

f. There is a temperature at which $CaCO_3$ (s) dissolves in water. Calculate this temperature. Is it possible for $CaCO_3$ to dissolve at this T?

Answers: a and b and c and d.

NaCl (s) --> Na⁺ (aq) + Cl⁻ (aq) ΔH_{f} -411 -239.66 -167.2 $\Delta H_{rxn} = [1(-239.66) + 1(-167.2)] - [(-411)] = 4.14 \text{ kJ/mole}$ 72.38 60.25 56.5 Sf $\Delta S_{rxn} = [1(60.25) + 1(56.5)] - [(72.38)] = 44.37 \text{ J/mole K}$ for ΔG_{rxn} , either use Hess' law or $\Delta G_{rxn} = \Delta H - T \Delta S$ Hess' law: ΔG_{f} -384 -261.87 -131.2 $\Delta G_{rxn} = [1(-261.87) + 1(-131.2)] - [(-384)] = -9.07 \text{ kJ/mole}$ OR $\Delta G_{rxn} = \Delta H - T \Delta S = 4,140 \text{ J/mole} - 298(44.37 \text{ J/mole K}) = -9080 \text{ J/mole} (compare to Hess' law)$ e. The temperature at which NaCl (s) does not dissolve in water: $\Delta G = \Delta H - T \Delta S.$ NOTE: ΔH and ΔS does NOT change with temperature but ΔG does. Set $\Delta G = 0 = 4,140 \text{ J/mole} - T (44.37 \text{ J/mole K})$ Solve for T = $93 \text{ K} = -180^{\circ}\text{C}$ Is it possible for NaCl not to dissolve at this T? No. Water is a solid, not liquid, at this T. $CaCO_3$ (s) $\rightarrow Ca^{2+}$ (aq) + CO_3^{2-} (aq) ΔH_{f} -1207 -543 -677 $\Delta H_{rxn} = [1(-543) + 1(-677)] - [(-1207)] = -12.9 \text{ kJ/mole}$ 92.9 Sf -53 -57 $\Delta S_{rxn} = [1(-53) + 1(-53)] - [(92.9)] = -202.9 \text{ J/mole K}$ for ΔG_{rxn} , either use Hess' law or $\Delta G_{rxn} = \Delta H - T \Delta S$ Hess' law: ΔG_{f} -528 -1128.8 -554 $\Delta G_{rxn} = [1(-554) + 1(-528)] - [(-1128.8)] = 46.8 \text{ kJ/mole}$ OR $\Delta G_{rxn} = \Delta H - T \Delta S = 12,900$ J/mole – 298(202.9 J/mole K) = 47,500 J/mole (compare to Hess' law) f. The temperature at which CaCO₃ (s) dissolves in water: $\Delta G = \Delta H - T \Delta S.$ NOTE: ΔH and ΔS does NOT change with temperature but ΔG does. Set ∆G = 0 = 12,900 J/mole – T (-202.9 J/mole K) Solve for T = $64 \text{ K} = -209^{\circ}\text{C}$ Is it possible for CaCO₃ to dissolve at this T? No. Water is a solid, not liquid, at this T. 3. You know water does not boil at 25° C under normal atmospheric (P = 1 atm) conditions. $H_2O(I) -> H_2O(g)$ a. Use Hess' law to calculate the numerical value of ΔH , ΔS , and ΔG for this reaction under standard state (298 K and 1 atm) conditions. (Answer: ΔH is greater than 0, ΔS is greater than 0, ΔG is greater than 0.) (i) This reaction is not favored by enthalpy because (ii) This reaction is favored by entropy because (iii) Is this reaction spontaneous at 25° C? What observation supports your answer? (iv) As temperature increases, does ΔG increase, decrease, or stay the same? b. Like you did in Question 2e, determine the temperature at which this reaction occurs. Use $\Delta G = \Delta H - T\Delta S$. (Answer: What is the boiling point of water?) Answers: $H_2O(I) --> H_2O(g)$ -241.8 ΔH_{f} -285.8 $\Delta H_{rxn} = [1(-241.8)] - [(-285.8)] = 44 \text{ kJ/mole} - endothermic. This amount of heat has to be supplied to evaporate 1 mole of$ water. Sf 188.8 -69.9 $\Delta S_{rxn} = [1(-69.9)] - [(188.8)] = 118.9$ J/mole K. Entropy increases – gas has higher entropy than liquid. for ΔG_{rxn} , either use Hess' law or $\Delta G_{rxn} = \Delta H - T \Delta S$ Hess' law: ΔG_{f} -237.2 -228.6 $\Delta G_{rxn} = [1(-228.6)] - [(-237.2)] = 8.6 \text{ kJ/mole}$. Water will not boil spontaneously at 25°C. OR $\Delta G_{rxn} = \Delta H - T \Delta S = 44,000 \text{ J/mole} - 298(118.9 \text{ J/mole K}) = 8,568 \text{ J/mole}$ (compare to Hess' law) (i) This reaction is not favored by enthalpy because $\Delta H > 0$. (ii) This reaction is favored by entropy because $\Delta S > 0$. (iii) This reaction is not spontaneous at 25°C because $\Delta G > 0$. (iv) As temperature increases, ΔG increase, decrease, or stay the same.

b. Determine the temperature at which this reaction occurs. Use $\Delta G = \Delta H - T\Delta S$. (Answer: What is the boiling point of water?)

 $\Delta G = \Delta H - T\Delta S$. NOTE: ΔH and ΔS does NOT change with temperature but ΔG does. Set $\Delta G = 0 = 44,000$ J/mole – T (118.9 J/mole K) Solve for T = 370 K = 97°C Compare this T to b.p. of water = 100°C.

4. Ideally, a fuel produces heat and work. Compare the combustion of octane (C_8H_{18} , the main component of gasoline in your car) and hydrogen (H_2 , thought by many to be the fuel fo the 21st century).

Determine the sign (+ or -) of $\Delta G,$ $\Delta H,$ $\Delta S,$ and w for each reaction.

a. Which fuel produces the most heat in kJ/g? Calculate ΔH in kJ/g for each fuel to support your answer. (Answer: hydrogen)

b. Which fuel produces the most work? Write a balanced chemical equation and compare moles of gas reactants to moles of gas products to support your answer.

c. Which reaction is favored by enthalpy?

d. Which reaction is favored by entropy?

e. Which fuel will combust at any temperature? For the other fuel, calculate the temperature at which combustion does <u>not</u> occur.

f. Why is octane a better fuel to use in a car engine?

g. The operating conditions in a heat engine (car engine) are high temperature and high pressure. As more reactants (fuel and air) are added to the engine, products are removed. Using your knowledge of thermodynamics, equilibrium, and reaction rate, explain why these T and P conditions are used.

h. Why is hydrogen not a good fuel to use in a car engine? (We'll discuss hydrogen fuel cells to produce electricity later in Chem 1B.)

Answers:

 1^{st} - balance the chemical equations. 2 C₈H₁₈ (I) + 25 O₂ (g) --> 16 CO₂ (g) + 18 H₂O (g)

 $2 H_2(g) + O_2(g) -> 2 H_2O(g)$

Then apply Hess' law to calculate ΔH in kJ/mole. Next, use the molar mass of the fuel to convert kJ/mole to kJ/g.

Fuel	Molar mass of fuel	∆H, kJ/mole	∆H, kJ/g	∆S, J/mole K	∆G, kJ/mole	Δn	W	T at which reaction occurs/not occurs
C ₈ H ₁₈ (I)	114	-5074	-44.5 favored by enthalpy	484 favored by entropy	-5200 spontane ous	9	< 0 work produced	Rxn ccurs at all T
H ₂ (g)	2	-241.8	-120.9 favored by enthalpy	-44.4 not favored by entropy	-229 spontane ous	-1	> 0 work supplied	Rxn does not occur at 5500 K

f. Octane is a better fuel to use in a car engine because this fuel produces heat and work. Hydrogen produces heat but not work.

g. The operating conditions in a heat engine (car engine) are high temperature and high pressure. As more reactants (fuel and air) are added to the engine, products are removed.

Thermodynamics – reaction produces heat and work. Higher T makes octane combustion more spontaneous (more negative Δ G). Higher P produces more work (w = -P Δ V).

Equilibrium – high T and P shifts reaction to reactant side since exothermic reaction and more gas products than gas reactants. Remove products (exhaust) shifts reaction toward product side.

Reaction rate – high T and P to make reaction go faster.

h. Hydrogen is not a good fuel to use in a car engine because Hydrogen produces heat but not work.

5. A stove designer decides to use a butane, C_4H_{10} , as a fuel for a stove. The butane is stored in a pressurized container and the pressurized butane is dispensed through a nozzle into the stove.

a. When butane and air are mixed together at room temperature and pressure, nothing happens. Give reasons.

b. Why is a spark needed for this combustion reaction to start?

c. Based on your observations of any combustion reaction, would you expect the rate constant for this reaction to be large or small? Give reasons.

d. Is the combustion of butane favored by entropy or enthalpy or both? Calculate ΔH and ΔS to support your answer.

e. As the temperature increases, does ΔG increase, decrease, or stay the same? Give reasons.

f. Some butane is released from the pressurized container (assume an adiabatic process). The temperature of the butane drops as it leaves the nozzle (goes to the lower pressure atmosphere from the high pressure container). Give reasons based on the 1st law of thermodynamics.

- 1st law of thermodynamics states the internal energy (E) can be converted to heat or work or both. Internal energy is the energy inside atoms and molecules due to the kinetic energy of the subatomic particles. If the internal energy increases (ΔE > 0), the temperature increases.
- Adiabatic process means q = 0.
- As butane gas leaves the nozzle, the gas expands. Is $\Delta V > 0$, < 0, or = 0? Then, use w = -p ΔV to determine if w > 0, < 0, or = 0.
- 1^{st} law of thermodynamics: $\Delta E = q + w$. Since q = 0 and w is _____, is $\Delta E > 0, < 0, \text{ or } = 0$?
- ΔE is _____ so temperature _____

g. As you know, a refrigerator is a heat engine that runs in reverse. Is the situation in part f a good way to run a refrigerator? Give reasons.

Answers:

a. Butane and air are not colliding with enough energy for bonds to break and form.

b. A spark is the energy needed for the butane and air to collide with enough energy for bonds to break and form. c. Large rate constant because a combustion reaction is fast.

d. 2 C_4H_{10} (I) + 13 O_2 (g) --> 8 CO_2 (g) + 10 H_2O (g)

 $\Delta H = -2660 \text{ kJ/mole} - \text{favored by enthalpy}$

 ΔS = 156 J/mole K – favored by entropy

e. $\Delta G = \Delta H - T\Delta S$. Since butane combustion is favored by enthalpy and entropy, higher T means more negative ΔG so ΔG decreases – reaction gets more spontaneous.

f. gas expands to $\Delta V > 0$ so w < 0 (work is produced).

 $\Delta E = q + w = 0 + (< 0) \text{ so } \Delta E < 0.$

 $\Delta E < 0$. Internal energy is the energy inside atoms and molecules, e.g., from electrons moving around nucleus) so if internal energy decreases, energy inside atoms and molecules decreases, e.g., move slower, and T decreases. g. No. See Objective 11 Practice Problem 8 on how refrigerators work. Butane is used in modern refrigerators.

6. Use thermo to determine storage temperature.

Hydrogen peroxide, H_2O_2 , is used as a disinfectant. H_2O_2 decomposes over time.

 $H_2O_2(I) ---> H_2O(I) + O_2(g)$

a. Calculate _____ to support the statement "H₂O₂ decomposes".

b. At what temperature should be H_2O_2 be stored so it does not decompose? (Hint: $\Delta H = -197 \text{ kJ}$, $\Delta S = 126 \text{ J/K}$ for this reaction)

c. You buy H_2O_2 at the store. Is the H_2O_2 decomposition reaction fast or slow?

d. Why is H₂O₂ stored in a brown bottle?

Answers:

a. Calculate $\Delta G = -234 \text{ kJ/mole at } 25^{\circ}\text{C}$.

b. $\Delta G = \Delta H - T \Delta S$.

NOTE: ΔH and ΔS does NOT change with temperature but ΔG does.

Set $\Delta G = 0 = -197,000 \text{ J/mole} - T (126 \text{ J/mole K})$

Solve for T = $-1570 \text{ K} = -1840^{\circ} \text{C}$. Can't have a T < 0K.

Hydrogen peroxide decomposes at all T because this reaction is favored by enthalpy and entropy.

Store H_2O_2 at a low T to slow rate of decomposition reaction.

c. Slow

d. Hydrogen peroxide decomposes faster in light. Brown bottle blocks light from H₂O₂.

7. A beverage is carbonated by dissolving CO_2 (g) into the drink:

CO₂ (g) ---> CO₂ (aq)

a. Carbonated beverages are _____ (acidic or basic or neutral) because CO_2 reacts with water to form H⁺ and HCO₃⁻: CO_2 (g) + H₂O (I) ---> H⁺ (aq) + HCO₃⁻ (aq) (2).

b. Does more CO₂ (g) dissolve in water (Reaction 1) or react with water (Reaction 2)? Calculate ΔG and K_{eq} at 25°C for each reaction to confirm your answer. (Answer: at 25°C, ΔG = 8 kJ/mole for Reaction 1 and ΔG = 45 kJ/mole for Reaction 2)

(1).

c. One way to keep the soda from going flat is to ____ (raise or lower) the temperature. Calculate ΔH for Reaction (1) and apply Le Chatelier's principle to confirm your answer. (Answer: at 25°C, ΔH is between -19 and -22 kJ/mole for Reaction 1)

d. What happens to K_{eq} for Reaction (1) as the temperature changes? Calculate K_{eq} at 0°C for Reaction (1) and compare to K_{eq} at 25°C for Reaction (1) to confirm your answer. (What equations do you want to use?)

e. Another way to keep the soda from going flat is to ____ (raise or lower) the pressure. Give reasons based on Le Chatelier's principle.

f. If the CO₂ (g) pressure is 1 atm, calculate the pH of the soda. (Hint: use Reaction 2 and $K_{eg} = [H^{+}(aq)][HCO_{3}^{-}]$ (aq)]/pressure of CO₂ (g). Answer: pH between 3.5 and 4.3) Answers: a. acidic b. $CO_2(g) ---> CO_2(aq)$ ΔG = 8.4 kJ/mole = 8400 J/mole = -RT In K_{eq}. Solve for K_{eq} at 25°C = 0.034 (use R = 8.31 J/mole K) $CO_2(g) + H_2O(I) ---> H^+(aq) + HCO_3^-(aq)$ ΔG = 44.7 kJ/mole = 44700 J/mole = -RT In K_{eq}. Solve for K_{eq} at 25°C = 1.45x10⁻⁸ (use R = 8.31 J/mole K) c. Keep the soda from going flat is to lower the temperature. CO_2 (g) ---> CO_2 (aq) $\Delta H = -19.4$ kJ/mole ==> exothermic Lower T (remove heat (a product)) and reaction shifts to product side – more CO₂ (aq) forms. d. To calculate K_{eq} at 0°C, calculate $\Delta G = \Delta H - T\Delta S$ at 0°C = 273 K. Then, use $\Delta G = -RT \ln K_{eq}$ with T = 273 K and solve for K_{eq} . CO_2 (g) ---> CO_2 (aq) ΔH = -19.4 kJ/mole and ΔS = -92.5 J/mole K. At T = 273 K, ∆G = -19400 J/mole – 173 (-92.5 J/mole K) = 5850 J/mole ΔG = -RT ln K_{eq} 5850 J/mole = -(8.31 J/mole K)(273 K) In K_{eq}. solve for $K_{eq} = 0.076$ at 0° C. K_{eq} at 25°C = 0.034 As T decreases, K increases == more CO₂ (g) dissolves in water. e. Keep the soda from going flat is to raise the pressure. CO_2 (g) ---> CO_2 (aq) 1 more gas reactant --> 0 moles gas product Raise pressure shifts reaction toward product side ==> more CO₂ (g) dissolves in water. $CO_2(g) + H_2O(I) ---> H^+(aq) + HCO_3^-(aq)$ K_{eq} at 25°C = 1.45x10⁻⁸ f. initial 1 0 0 reacts x х $K_{eq} = [H^+ (aq)][HCO_3^- (aq)]/pressure of CO_2 (g).$ Х Х $K_{eq} = (x)(x)/1 = 1.45 \times 10^{-1}$ equilibrium 1 - x Х Х Х assume 1-x = 1 since K_{eq} is very small Solve for $x = [H^+ (aq)] = 1.2x10^{-4}$. $pH = -log [H^+ (aq)] = -log (1.2x10^{-4}) = 3.9$

8. One way to make a non-spontaneous reaction occur is to change the temperature. Another way to make a non-spontaneous reaction occur is to use the energy from a spontaneous reaction.

Lime stains (Ca(OH)₂) make your glasses and cups look dirty although they may be clean.

a. $Ca(OH)_2$ (s) <==> Ca^{2^+} (aq) + 2 OH^- (aq) $K_{sp} = 4.7 \times 10^{-6}$.

Calculate ΔG for this reaction. (Hint: use $\Delta G = -RT \ln K_{eq}$)

b. You can use acid, like HCl, to remove (dissolve) an insoluble hydroxide solid. Complete the chemical equation and then write a net ionic equation.

Ca(OH)₂ (s) + HCl ---->

c. Add Equation (1) to Equation (2) to get Equation (3). Equation (3) should be the same as your net ionic equation in part b.

 $\begin{array}{c} Ca(OH)_{2} (s) <==> Ca^{2^{+}} (aq) + 2 OH^{-} (aq) & K_{sp} = 4.7 \times 10^{-6} \\ 2 H^{+} (aq) + 2 OH^{-} (aq) <==> 2 H_{2}O (I) & K = 1/K_{w}^{-2} = 1 \times 10^{28} \\ d. Calculate K for Equation (3). How does K show acid dissolves lime stains? \end{array}$ (1)

e. Calculate Δ G for Equation (3). How does Δ G show acid dissolves lime stains? Answers:

a. $\Delta G = -RT \ln K_{eq} = -(8.31 \text{ J/mole K})(298 \text{ K}) \ln (4.7x10^{-6}) = 30400 \text{ J/mole}$ b. $Ca(OH)_2 (s) + 2 \text{ HCI} ----> CaCl_2 (aq) + 2 H_2O (l)$ $Ca(OH)_2 (s) + 2 \text{ H}^+ + 2 \text{ CI}^- ---> Ca^{2^+} + 2 \text{ CI}^- (aq) + 2 H_2O (l)$ Net ionic equation: $Ca(OH)_2 (s) + 2 \text{ H}^+ ----> Ca^{2^+} (aq) + 2 H_2O (l)$ b. $Ca(OH)_2 (s) <===> Ca^{2^+} (aq) + 2 -OH^- (aq)$ $K_{sp} = 4.7x10^{-6}$ (1) $2 \text{ H}^+ (aq) + 2 -OH^- (aq) <===> 2 H_2O (l)$ $K = 1/K_w^2 = 1x10^{28}$ (2) $Ca(OH)_2 (s) + 2 \text{ H}^+ ----> Ca^{2^+} (aq) + 2 H_2O (l)$ (3) d. K for Reaction (3) = K for Reaction (1) x K for Reaction (2) $= (4.7x10^{-6}) (1x10^{28})$

= $(4.7 \times 10^{-6}) (1 \times 10^{28})$ = 4.7×10^{22} ==> This reaction occurs! Acid dissolves lime stains.

e. ΔG = -RT In K_{eq} = -(8.31 J/mole K)(298 K) In (4.7x10²²) = -129000 J/mole ==> This reaction occurs! Acid dissolves lime stains.

9. Biology: ATP is the universal currency of energy in biological systems. We use ATP in our bodies to supply energy for other reactions to occur. The hydrolysis of ATP to ADP and orthophosphate is a **spontaneous** reaction with a ΔG of -7.3 kcal/mole:

ATP + H_2O -----> ADP + P_1 + H^+ $\Delta G = -7.3$ kcal/mole (1)

where P_1 is orthophosphate, HPO_4^{2-} .

One of the ways metabolic energy is produced is by glycolysis. In glycolysis, glucose is converted into pyruvate in a 10 step process. In the first step, glucose is phosphorylated to glucose 6-phosphate:

(2).

 $\Delta G = 3.3$ kcal/mole glucose + P_i ----> glucose 6-phosphate + H_2O

a. Does the reaction that converts glucose to glucose 6-phosphate (Reaction 2) occur spontaneously? Give reasons.

b. (i) Add Reaction (1) to Reaction (2). Write the sum of the two reactions to give Reaction (3).

(Answer: glucose + ATP -----> glucose 6-phosphate + ADP + H^+)

(ii) Calculate the ΔG and K for Reaction (3). Does Reaction (3) occur spontaneously? Give reasons.

c. Explain why ATP is needed for the first step of glycolysis to occur.

d. Does Reaction (3) produce more products if the pH increases? Give reasons.

Answers:

a. No. $\Delta G > 0$ so glucose to glucose 6-phosphate is not spontaneous.

ATP + H_2O -----> ADP + P_i + H^+ b.

 $\Delta G = -7.3$ kcal/mole (1) glucose + P_i -----> glucose 6-phosphate + H_2O $\Delta G = 3.3 \text{ kcal/mole}$ (2). Sum: ATP + glucose -----> ADP + glucose 6-phosphate + H⁺ $\Delta G = \Delta G_1 + \Delta G_2 = -7.3 + 3.3 = -4.0$ kcal/mole $\Delta G = = -4.0$ kcal/mole x 4.18 J/1 cal = -16.7 kJ/mole

 $\Delta G = -RT \ln K_{eq}$.

-16700 J/mole = -(8.31 J/mole K)(298 K) ln (K_{eq}). Solve for K_{eq} =

 $\Delta G < 0$ so this reaction is spontaneous.

c. The energy from the ATP hydrolysis reaction is needed (supplied) to make the glucose to glucose 6-phosphate occur. d. As pH increase, H+ decreases and reaction shifts to product side and produces more products.