Objective 7. Understand equilibrium reactions (equilibrium constant, LeChatelier's principle, equilibrium calculation).

1. Hydrogen iodide is a stronger acid than HCl and is produced according to the equation H_2 (g) + I_2 (g) ----> 2 HI (g).
a. A partial equilibrium constant expression for this reaction is given. What is the numerical value of x, y, and z?
$K_{eq} = [HI]^x/[H_2]^y [I_2]^z$
b. K_{eq} = 64 at 400°C. Will there be more HI present at equilibrium or more H_2 and I_2? Give reasons.
c. LeChatelier's application:
If more H_2 is added the reaction shifts toward products. In other words, more products are produced to re-establish equilibrium.
Add H_2 so $[HI]^2/[H_2] [I_2]$ decreases below K_{eq} = 64. To get the ratio of $[HI]^2/[H_2] [I_2]$ back to 64, the reaction has to form more products (numerator) so the reaction shifts towards products.
(i) If HI (g) is added, the reaction shifts to make more reactants (goes in reverse direction). Does the ratio of $[HI]^2/[H_2] [I_2]$ increase or decrease? To get this ratio back to 64, does the numerator or denominator have to decrease?
(ii) If HI (g) is removed, does the ratio of $[HI]^2/[H_2] [I_2]$ increase or decrease? To get this ratio back to 64, does the numerator or denominator have to decrease? Which direction does the reaction shift?
(iii) If I_2 (g) is added, does the ratio of $[HI]^2/[H_2] [I_2]$ increase or decrease? To get this ratio back to 64, does the numerator or denominator have to decrease? Which direction does the reaction shift?
(iv) If H_2 (g) is removed, does the ratio of $[HI]^2/[H_2] [I_2]$ increase or decrease? To get this ratio back to 64, does the numerator or denominator have to decrease? Which direction does the reaction shift?
(v) If the reaction pressure is raised, the reaction will not shift to either side. An increase in pressure is like an increase in concentration of each gas. Explain why an increase in pressure does shift the reaction.
d. ΔH for this reaction is -9.4 kJ/mole. If the reaction temperature is raised, will reaction shift to reactants or products? (Hint: is this reaction exothermic or endothermic? Is heat a reactant or product in this reaction? If the reaction temperature increases, think of it as adding heat.)
e. If the reaction temperature is raised, the numerical value of K decreases. Explain why K decreases. (Hint: relate your answer to part d.)
f. Equilibrium calculation: 1 mole of H_2 and 1 mole of I_2 are placed in a 1 liter container at 400°C. The reaction occurs. Calculate the equilibrium concentrations of each reactant and product.

	H_2 (g) +	I_2 (g) ----->	2 HI (g)
initial	1	1	0
reacts	x	x	2x
equilibrium	1-x	1-x	2x

Substitute into K_{eq} expression from Question 1a: $K_{eq} = 64 = [HI]^2/[H_2] [I_2] = (2x)^2/(1-x)(1-x)$
Solve for x: $64(1-x)(1-x) = 4x^2$
$60 x^2 – 128x + 64 = 0$
Use quadratic equation: x = 1.3 and 0.8
x can't be 1.3 because $[H_2]$ and $[I_2]$ would be less than 0 at equilibrium.
So x = 0.8, which means $[H_2] = 1 – 0.8 = 0.2$ and $[I_2] = 1 – 0.8 = 0.2$ and $[HI] = 2 (0.8) = 1.6$ at equilibrium.
This makes sense since K_{eq} = 64, there should be more products than reactants.

2. Hydrogen iodide decomposes according to the equation 2 HI (g) ---> H_2 (g) + I_2 (g).
a. Write an equilibrium constant expression for this reaction: K_{eq} =
b. K_{eq} = 0.0156 at 400°C. Will there be more HI present at equilibrium or more H_2 and I_2? Give reasons.
c. LeChatelier's application:
(i) If H_2 (g) is removed, which direction does the reaction shift?
(ii) If the reaction pressure is raised, which direction does the reaction shift?
d. ΔH for this reaction is 9.4 kJ/mole. If the reaction temperature is raised, will reaction shift to reactants or products?
e. If the reaction temperature is raised, will K increase or decrease?
f. Equilibrium calculation: 1 mole of HI is placed in a 1 liter container at 400°C. The reaction occurs. Calculate the equilibrium concentrations of each reactant and product.

	2 HI (g) --->	H_2 (g) + I_2 (g).
initial	1	
reacts		
equilibrium		

3. Under the conditions of a car engine, nitrogren and oxygen reacts to form NO_x, which is a component of smog:
N_2 (g) + O_2 (g) --> 2 NO (g)
N_2 (g) + 2 O_2 (g) --> 2 NO_2 (g)
a. For each reaction, write an equilibrium constant expression.
b. Under what temperature (low T or high T) and pressure (low P or high P) conditions does each reaction occur? Give reasons based on LeChatelier's principle.

4. Dinitrogen tetroxide, N_2O_4, is a colorless gas that boils at 21°C. As a gas, it is extensively dissociated to NO_2. As a liquid, it is partly dissociated to NO_2. NO_2 is a reddish-brown toxic gas that makes up part of the brown cloud in Southern California and Denver during the winter months. (Reddish-brown toxic NO_2 gas gets trapped in lower atmosphere due to temperature inversion in winter in which less dense warm air traps more dense cold air beneath it.)

N_2O_4 (g) <==> 2 NO_2 (g)

a. Write an equilibrium constant expression.
b. At 25°C, 1.00 mole N_2O_4 is placed in a 1.0 liter container. At equilibrium, the container has 0.28 mole NO_2 present. Calculate a numerical value for K_{eq}.
c. At 25°C, the gas inside the container is reddish-brown. When this container is placed in an ice bath, the gas is colorless. Is the dissociation of N_2O_4 exothermic or endothermic? Explain. Calculate the heat of reaction to confirm your answer.

5. The Haber process is the industrial process for the synthesis of ammonia (NH_3) from N_2 and H_2. In this process, the reaction conditions are high pressure and low temperature. A catalyst is used and product is removed from the reaction vessel during the reaction.
a. Write a balanced chemical equation that represents this reaction.
b. Write an equilibrium constant expression.
c. Explain why these reaction conditions (high pressure, low temperature, catalyst is used, and product is removed) are used. If a catalyst was not used, could a higher reaction be used to optimize the yield? Give reasons.

6. Drano drain cleaner consists of Al filings and NaOH pellets. When water is added, the heat produced melts and saponifies the fat that clogs a drain.

2 Al (s) + 2 NaOH (s) + 6 H_2O (l) --> 2 $NaAl(OH)_4$ (aq) + 3 H_2 (g)

a. Write an equilibrium constant expression.
b. Would you expect this reaction to have a large K or small K? Explain.
c. In terms of reactants and products, explain how this reaction can be shifted to the right (toward products).
d. If an excess amount of water is added, how will the reaction be affected?
e. If hot water was added instead of cold water, would Drano work better? In other words, which direction would the reaction shift?
f. If the drain was plugged immediately after Drano was added to the clog, would Drano work better? In other words, which direction would the reaction shift?

7. In Lab 1, an alcohol reacts with a carboxylic acid to produce an ester and water. This reaction is an exothermic, equilibrium reaction and is catalyzed with sulfuric acid.
a. Draw a reaction energy diagram for this reaction with and without the catalyst. Label ΔH and the activation energy on your diagram.
b. Two ways to increase the reaction rate are to raise the temperature and to use a catalyst. Why is a catalyst used in the esterification reaction instead of heating the reaction for an hour at 100°C?
c. Draw a graph that shows the concentration of acid vs. time of reaction and the concentration of ester vs. time of reaction. What happens to the reaction rate as a reaction proceeds?