Chem 1314
During Class Invention
Spring 2007

Name___________________________
TA Name _______________________
Lab Section #______

1. The reaction

$$H_{2(g)} \quad + \quad I_{2(g)} \quad \rightleftharpoons \quad 2HI_{(g)}$$

occurs in a 1.0 L container at a given temperature. Initially the concentration of $[H_2]$ and $[I_2]$ are both 0.350 M. In the table below are the results of 6 successive measurements where the concentration of each species in the reaction is provided.

Measurement #	$[H_2]$ (M)	$[I_2]$ (M)	[HI] (M)	Ratio $\frac{[HI]^2}{[H_2][I_2]}$
1	0.350	0.350	0	0
2	0.255	0.255	0.190	**0.555**
3	0.155	0.155	0.390	**6.33**
4	0.0900	0.0900	0.520	**33.4**
5	0.0775	0.0775	0.545	**49.5**
6	0.0775	0.0775	0.545	**49.5**

Calculate the magnitude of the reaction quotient, $\frac{[HI]^2}{[H_2][I_2]}$, for each measurement and enter the value into the appropriate cell in the table above. (Show at least one of the calculations here.)

Measurment #2: $\mathbf{\frac{[HI]^2}{[H_2][I_2]} = \frac{[0.190]^2}{[0.255][0.255]} = 0.555}$

Measurment #3: $\mathbf{\frac{[HI]^2}{[H_2][I_2]} = \frac{[0.390]^2}{[0.155][0.155]} = 6.33}$

Measurment #4: $\mathbf{\frac{[HI]^2}{[H_2][I_2]} = \frac{[0.520]^2}{[0.0900][0.0900]} = 33.4}$

Measurment #5 : $\mathbf{\frac{[HI]^2}{[H_2][I_2]} = \frac{[0.545]^2}{[0.0775][0.\ 0775]} = 49.5}$

Measurment #6 : $\mathbf{\frac{[HI]^2}{[H_2][I_2]} = \frac{[0.545]^2}{[0.0775][0.\ 0775]} = 49.5}$

a. What is happening to the value of the reaction quotient moving from Exp.#1 to Exp. #5?

The value of the reaction quotient gets larger for each experiment until Exp. #5 (and #6) where equilibrium is established.

b. For Exp. #4 what is the concentration of $[H_2]$ and $[I_2]$ reacting?

	$H_2(g)$ +	$I_2(g)$ ⇌	$2HI(g)$
Initial	**0.350 M**	**0.350 M**	**0**
Change	**- x**	**- x**	**+2x**
Equilibrium	**0.0900**	**0.0900**	**0.520**

For $[H_2]$ and $[I_2]$ the amount reacting is x,. In Exp. #4 x = 0.350 – 0.0900 = 0.260 M and the ICE table would look like,

	$H_2(g)$ +	$I_2(g)$ ⇌	$2HI(g)$
Initial	**0.350 M**	**0.350 M**	**0**
Change	**- 0.260**	**-0.260**	**+0.520**
Equilibrium	**0.0900**	**0.0900**	**0.520**

c. For Exp. #4 what is the concentration of [HI] formed?

See the ICE table above. The [HI] formed is 0.520 M

d. Explain the relationship between the concentration of $[H_2]$ and $[I_2]$ reacting and the concentration of [HI] formed?

That relationship come from the stoichiometry of the balanced chemical equation. For this reaction 1 mol of H_2 and 1 mol of I_2 react to produce 2 mol of HI.

e. What is happening in Exp. #5 and #6?

In Exp. #5 and #6 the amounts of $[H_2]$, $[I_2]$ and [HI] are constant. This would indicate that equilibrium had been established at Exp #5. Once equilibrium is established, even though the reaction is still occurring there is no change in $[H_2]$, $[I_2]$ and [HI].

f. What is the magnitude of the equilibrium constant for this reaction?

Measurment #5: $$\frac{[HI]^2}{[H_2][I_2]} = \frac{[0.545]^2}{0.0775][0.0775]} = 49.5 = K$$

g If Exp. #7 and #8 were performed, what would you expect the reaction quotient to be?

Since the reaction has attained equilibrium at Exp.5, any additional experiments will have the same amounts of $[H_2]$, $[I_2]$ and [HI] as Exp. #5. So the reaction quotient will still have a value of 49.5.

2. The reaction

$$\mathrm{NOBr}(g) \rightleftharpoons \mathrm{NO}(g) + \tfrac{1}{2}\,\mathrm{Br_2}(g)$$

has been carefully studied at 350 ˚C and the K_c is 0.079. Which direction will the reaction proceed to establish equilibrium under each of the following initial conditions?

i) $[NOBr]_o = 0.100$ M : $[NO]_o = 0$: $[Br_2]_o = 0$

To determine the direction the reaction proceeds to establish equilibrium the value of Q, the reaction quotient, is compared to K_c. The reaction quotient is,

$$Q = \frac{[NO]_{initial}[Br_2]_{initial}^{1/2}}{[NOBr]_{initial}} = \frac{[NO]_o[Br_2]_o^{1/2}}{[NOBr]_o}$$

For the set of conditions

$$Q = \frac{(0)(0)^{1/2}}{0.100} = 0$$

To determine the direction the reaction will proceed Q is compared to K_c. In this case $Q < K_c$. In order for Q to equal K_c the concentration of NO and Br_2 must increase and the concentration of NOBr must decrease. So the reaction proceeds from left-to-right.

ii) $[NOBr]_o = 0$: $[NO]_o = 0.100$ M : $[Br_2]_o = 0.100$ M

The reaction quotient is,

$$Q = \frac{[NO]_{initial}[Br_2]_{initial}^{1/2}}{[NOBr]_{initial}} = \frac{[NO]_o[Br_2]_o^{1/2}}{[NOBr]_o}$$

For the set of conditions

$$Q = \frac{(0.100)(0.100)^{1/2}}{0} = \text{undefined}$$

(Q is very large, if [NOBr] is close to 0.)

To determine the direction the reaction will proceed Q is compared to K_c. In this case $Q > K_c$. In order for Q to equal K_c the concentration of NO and Br_2 must decrease and the concentration of NOBr must increase. So the reaction proceeds from right-to-left.

iii) $[NOBr]_o = 0.100$ M : $[NO]_o = 0$: $[Br_2]_o = 0.100$ M

The reaction quotient is,

$$Q = \frac{[NO]_{initial}[Br_2]_{initial}^{1/2}}{[NOBr]_{initial}} = \frac{[NO]_o[Br_2]_o^{1/2}}{[NOBr]_o}$$

For the set of conditions

$$Q = \frac{(0)(0.100)^{1/2}}{0.100} = 0$$

To determine the direction the reaction will proceed Q is compared to K_c. In this case $Q < K_c$. In order for Q to equal K_c the concen-tration of NO and Br_2 must increase

and the concentration of NOBr must decrease. So the reaction proceeds from left-to-right.

iv) $[NOBr]_o = 0.100$ M : $[NO]_o = 0.100$ M : $[Br_2]_o = 0.100$ M

$$\mathbf{Q = \frac{[NO]_o[Br_2]_o^{1/2}}{[NOBr]_o} = \frac{(0.1)(.1)^{1/2}}{0.1} = .316 : Q > K_c : L \leftarrow R}$$

v) $[NOBr]_o = 0.200$ M : $[NO]_o = 0.0500$ M : $[Br_2]_o = 0.100$ M

$$\mathbf{Q = \frac{[NO]_{initial}[Br_2]_{initial}^{1/2}}{[NOBr]_{initial}}}$$

$$\mathbf{Q = \frac{(0.05)(.1)^{1/2}}{0.2} = .079 : Q = K_c}$$

reaction is at equilibrium so no change occurs

1a. State Le Chatelier's principle.

If a chemical reaction at equilibrium is subjected to a change in conditions that displaces it from equilibrium, then the reaction proceeds toward a new equilibrium state in the direction that offsets the change in conditions.

b. Identify three factors which can affect a reaction at equilibrium. Using examples discussed in lecture, briefly describe how each factor can affect a reaction at equilibrium.

1. Concentration of a reactant or product

When a system is at equilibrium, increasing the concentration of a reactant or product will cause the reaction to re-establish equilibrium by shifting the reaction in a direction which relieves the stress. For example, in the simulation reaction,

$$A_2(g) \quad + \quad B_2(g) \quad \rightleftharpoons \quad 2AB(g)$$

When the reaction is at equilibrium and the $[B_2]$ is increased the reaction proceeds from left-to-right to relieve the stress. When B_2 is added the reaction shifts in a direction to relieve the stress, by trying to decrease the amount of B_2. So the reactions proceeds from left-to-right. Similarly when the reaction is at equilibrium, addition of AB shifts the reaction from right-to-left to relieve the stress.

2. Reaction volume or pressure

To understand the effect of volume on a reaction, consider the following reaction.

$$PCl_5(g) \rightleftharpoons PCl_3(g) + Cl_2(g)$$

Assume the reaction is at equilibrium in a sealed container. If the volume of the reaction container is lowered, molecules in the container are pushed closer together and the internal pressure increases. To relieve this stress the reaction shifts in the direction to decrease the crowding of the molecules. It proceeds from right to left because the left side of the reaction has fewer gas molecules compared to the right.

If the volume is increased the reaction proceeds from left-to-right. The increase in volume means there are fewer molecules per unit volume and the reaction proceeds in a direction to increase the number of molecules per unit volume and thus maintain constant pressure.

3. Temperature

To understand how temperature effects a reaction at equilibrium consider the equilibrium of NO_2 and N_2O_4. The reaction is endothermic;

$$\text{heat} + N_2O_4(g) \rightleftharpoons 2NO_2(g)$$

colorless orange-brown

When the reaction is cooled the color of the sample becomes lighter, indicating more $N_2O_4(g)$ was formed. Heat is removed from the reaction system when the reaction is cooled. As the reaction is cooled it proceeds in the direction to offset the stress, in a direction to produce heat, from right to left. In general for endothermic reactions decreasing the temperature shifts the equilibrium towards the left and adding heat shifts the equilibrium to the right. It is just the opposite for exothermic reactions.

c. The reaction

$$2H_2S(g) + 3O_2(g) \rightleftharpoons 2H_2O(g) + 2SO_2(g)$$

has a ΔH = -1036 kJ. Given the reaction is at equilibrium, predict the direction the reaction will shift when disrupted by each of the following

i)the amount of H_2O is increased
reaction will shift from right to left (←)

ii)the temperature of the reaction is increased
reaction will shift from right to left (←)

iii)the volume of the container is decreased
reaction will shift from left to right(→)

iv)the amount of H_2S is decreased
reaction will shift from right to left (←)

2. Define the non-equilibrium reaction quotient, Q, and explain how it can be used to predict the direction a reaction will proceed to establish equilibrium.

The reaction quotient for the chemical reaction,

$$aA(g) + bB(g) \rightleftharpoons cC(g) + dD(g)$$

is defined as,

$$Q = \frac{[C]^c[D]^d}{[A]^a[B]^b}$$

The concentration used in the quotient, can be nonequilibrium concentrations. When equilibrium concentrations are used $Q = K_c$.

The direction the reaction will proceed to establish equilibrium depends on the comparison of the magnitudes of Q and K_c.