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CHEMICAL EQUILIBRIUM

Writing Equilibrium Expressions

In order to write the equilibrium expression for a system in a state of equilibrium you need to know:

- the balanced equation for the reaction
- the phases (solid, liquid, gas, or dissolved) of each species involved in the reaction.

Writing Expressions for K_c

The general equilibrium expression for a reaction:

$$aA + bB \leftrightarrows cC + dD$$

is written as:

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

The brackets "[ ]" represent the concentration of the species (moles per liter or molarity). "a, b, c, and d" represent the coefficients used to balance the equation. The "c" in K_c indicates that the value of K is determined using the concentrations of each species.
There are two cases when a species is not shown in the equilibrium expression:

- when it is a solid
- when it is a pure liquid or solvent

Writing Expressions for K_p

When one or more of the species in a system exists in the gaseous phase, the partial pressure of that species can be used in the equilibrium expression Dissolved species are still expressed as moles per liter (molarity).

Examples

Examples of equilibrium expressions K_c for a variety of equilibrium systems follow. When one or more gaseous substances are involved, the K_p expression is also given.

- The production of ammonia from nitrogen and hydrogen gases.

$$N_2(g) + 3\,H_2(g) \leftrightarrows 2\,NH_3(g)$$

$$K_c = \frac{[NH_3]^2}{[N_2][H_2]^3}$$

$$K_p = \frac{P^2_{(NH3)}}{P_{(N2)}P^3_{(H2)}}$$

- The thermal decomposition of calcium carbonate.

$$CaCO_3(s) \leftrightarrows CaO(s) + CO_2(g)$$

$$K_c = [CO_2]$$
$$K_p = P_{(CO2)}$$

- The oxidation-reduction reaction occuring between iron(III) chloride and tin(II) chloride.

$$2\ FeCl_3(aq) + SnCl_2(aq) \leftrightarrows 2\ FeCl_2(aq) + SnCl_4(aq)$$

$$K_c = \frac{[FeCl_2]^2[SnCl_4]}{[FeCl_3]^2[SnCl_2]}$$

- The replacement of silver ions by copper.

$$Cu(s) + 2\ Ag^+(aq) \leftrightarrows Cu^{2+}(aq) + 2\ Ag(s)$$

$$K_c = \frac{[Cu^{2+}]}{[Ag^+]^2}$$

- The interaction of acetic acid with water.

$$CH_3COOH(aq) + H_2O(l) \leftrightarrows H_3O^+(aq) + CH_3COO^-(aq)$$

$$K_c = \frac{[H_3O^+][CH_3COO^-]}{[CH_3COOH]}$$

- The reaction of carbon dioxide gas with a sodium hydroxide solution.

$$CO_2(g) + NaOH(aq) \leftrightarrows NaHCO_3(aq)$$

$$K_c = \frac{[NaHCO_3]}{[CO_2][NaOH]}$$

$$K_p = \frac{[NaHCO_3]}{P_{(CO2)}\,[NaOH]}$$

- The evaporation of water.

$$H_2O(l) \leftrightarrows H_2O(g)$$

$$K_c = [H_2O(g)]$$

$$K_p = P_{(H2O)}$$

MAKING AN ICE CHART
AN AID IN SOLVING EQUILIBRIUM PROBLEMS

❑ An useful tool in solving equilibrium problems is an ICE chart.

- "I" stands for the initial concentrations (or pressures) for each species in the reaction mixture.
- "C" represents the change in the concentrations (or pressures) for each species as the system moves towards equilibrium.
- "E" represents the equilibrium concentrations (or pressures) of each species when the system is in a state of equilibrium.

- How to make an ICE chart
- Sample ICE charts
    - Only reactant species are present initially
    - Only product species are present initially
    - Species added to a system initially in a state of equilibrium
    - Gaseous species and K_p

How to Make an ICE Chart

In making an ICE chart the following items should be noted:

- Express all quantities in terms of **MOLARITY** (moles per liter). (If using K_p, gaseous species must be expressed in appropriate pressure units.)
- Use **initial quantities** when calculating the reaction quotient, Q, to determine the direction the reaction shifts to establish equilibrium.
- Use **equilibrium quantities** in calculations involving the equilibrium constant, K.
- The **change in each quantity** must be in agreement with the **reaction stoichiometry.**
- Read each problem carefully to identify what quantities are given, including their unit of measure, and to identify what is unknown.

- Clearly define the change you choose to be represented by "x." Define all other unknown changes in terms of this change.

The following is a "how to" make an ICE chart using the example to illustrate the process.

Example: A mixture consisting initially of 3.00 moles NH_3, 2.00 moles of N_2, and 5.00 moles of H_2, in a 5.00 L container was heated to 900 K, and allowed to reach equilibrium. Determine the equilibrium concentration for each species present in the equilibrium mixture.

$$2\ NH_3(g) \leftrightarrows N_2(g) + 3\ H_2(g) \quad K_c = 0.0076\ @\ 900\ K$$

- Convert the initial quantities to molarities as shown for NH_3.

$$\frac{3.00 \text{ moles } NH_3}{5.00 \text{ L}} = 0.600 \text{ M}$$

- Create a chart as illustrated below and enter in the known quantities.

	NH_3	N_2	H_2
Initial Concentration (M)	0.600	0.400	1.00
Change in Conc. (M)			
Equilibrium Conc. (M)			

- Calculate Q_c and compare to K_c to determine the direction the reaction will proceed.

$$Q_c = \frac{[N_2][H_2]^3}{[NH_3]^2} = \frac{(0.400)(1.00)^3}{(0.600)^2} = 1.11$$

$$K_c < Q_c \text{ reaction will proceed towards the left}$$

- Assign a variable "x" that represents the change in the amount of one of the species. The species with the lowest coefficient in the balanced equation usually is the easiest to handle when it comes to doing the math. Here let "x" = change in the amount of N_2.
- Determine the change in all the other species in terms of "x." Remember the change must be in agreement with the stoichiometry of the balanced equation, in this case 2:1:3. Since the reaction goes in the reverse direction the concentrations of N_2 and H_2gases will decrease (note the negative sign) and that of NH_3 will increase. Put these quantities into the chart (shown in red).

	NH_3	N_2	H_2
Initial Concentration (M)	0.600	0.400	1.00
Change in Conc. (M)	+ 2 x	- x	- 3 x
Equilibrium Conc. (M)			

- Express the equilibrium concentrations in terms of "x" and the initial amounts (shown in green).

	NH_3	N_2	H_2
Initial Concentration (M)	0.600	0.400	1.00
Change in Conc. (M)	+ 2 x	- x	- 3 x
Equilibrium Conc. (M)	0.600 + 2 x	0.400 - x	1.00 - 3 x

- Substitute the expressions for the equilibrium concentration into the expression for the equilibrium constant and solve for "x." Once x is known, the equilibrium concentration for each species can be calculated.

$$\frac{[N_2][H_2]^3}{[NH_3]^2} = \frac{(0.400 - x)(1.00 - 3x)^3}{(0.600 + 2x)^2} = 0.0076$$

$$x = 0.21575 = 0.216$$

$$[N_2] = 0.400 - 0.216 = 0.184 \text{ M}$$
$$[H_2] = 1.00 - 3(0.216) = 0.352 \text{ M}$$
$$[NH_3] = 0.600 + 2(0.216) = 1.032 \text{ M}$$

The value of x was determined using the method of successive approximations.

❑ **SAMPLE ICE CHARTS**

The following examples illustrating writing ICE charts for the problems given. Although each problem appears to be "different" the process for creating the ICE chart is the same.

- Only reactant species are present initially
- Only product species are present initially
- Species added to a system initially in a state of equilibrium
- Gaseous species and Kp

Only Reactant Species Are Present Initially

Example: 4.00 moles of HI are placed in an evacuated 5.00 L flask and then heated to 800 K. The system is allowed to reach equilibrium. What will be the equilibrium concentration of each species?

$$2\,HI(g) \leftrightarrows H_2(g) + I_2(g) \quad K_c = 0.016 \text{ @ } 800 \text{ K}$$

Let "x" represent the change in concentration of the hydrogen gas. Since we start with HI alone, the reaction must proceed to the right resulting in an increase in the amount of hydrogen gas.

	$HI(g)$	$H_2(g)$	$I_2(g)$
Initial Concentration (M)	0.800	0	0
Change in Concentration (M)	- 2 x	+ x	+ x
Equilibrium Concentration (M)	0.800 - 2 x	0 + x	0 + x

Only Product Species Are Present Initially

Example: 0.600 moles of NO and 0.750 moles of O_2 are placed in an empty 2.00 L flask. The system is allowed to establish equilibrium. What will be the equilibrium concentration of each species in the flask?

$$2\ NO_2(g) \leftrightarrows 2\ NO(g) + O_2(g) \quad K_c = 0.50$$

Let "x" represent the change in concentration of the oxygen gas. Since only NO and O_2 are present, the reaction must proceed to the left in order to establish equilibrium. The O_2 gas will decrease in concentration over time.

	$NO_2(g)$	$NO(g)$	$O_2(g)$
Initial Concentration (M)	0	0.300	0.375
Change in Concentration (M)	+ 2 x	- 2 x	- x
Equilibirum Concentration (M)	2 x	0.300 - 2 x	0.375 - x

Species Added to a System Initially in a State of Equilibrium

Example: The concentrations of an equilibrium mixture of O_2 , CO, and CO_2 were 0.18 M, 0.35 M, and 0.029 M respectively. Enough CO was added to the flask containing the equilibrium mixture to momentarily raise its concentration to 0.60 M. What will be the concentration of each species in the flask once equilibrium has been re-established after the additional carbon monoxide was added?

$$2\ CO_2(g) \leftrightarrows 2\ CO(g) + O_2(g)$$

After the addition of more CO the system is no longer in equilibrium. The once equilibrium quantities of the other three substances are now initial quantities. Let "x" represent the change in the amount of O_2 gas. Adding the CO will force the reaction to proceed in the reverse direction ($K < Q$) causing the amount of O_2 to decrease. (Note: The equilibrium quantities given in the problem, before the addition of more CO, are also used to calculate the value of the equilibrium constant, K_c.)

	$CO_2(g)$	$CO(g)$	$O_2(g)$
Initial Concentration (M)	0.029	0.60	0.18
Change in Concentration (M)	+ 2 x	- 2 x	- x
Equilibrium Concentration (M)	0.029 + 2 x	0.60 - 2 x	0.18 - x

Gaseous Species and K_p

Example: Cl_2 gas undergoes homolytic cleavage into chlorine atoms at 1100°C. K_p at 1100°C for this process is 1.13×10^{-4}. If a sample with an initial Cl_2 gas pressure of 0.500 atm was allowed to reach equilibrium, what is the total pressure in the flask?

$$Cl_2(g) \leftrightarrows 2\ Cl(g)$$

Let "x" represent the change in the pressure of the Cl_2 gas. Since the reaction will proceed forwards to establish equilibrium the pressure of the Cl_2 gas will decrease. The total pressure at equilibrium will equal the sum of the partial pressures of each gas at equilibrium.

	$Cl_2(g)$	$Cl(g)$
Initial Pressure (atm)	0.500	0
Change in Pressure (atm)	- x	+ 2 x
Pressure at Equilibrium (atm)	0.500 - x	0 + 2 x

❑ CALCULATING EQUILIBRIUM CONSTANTS

We need to know two things in order to calculate the numeric value of the equilibrium constant:

- the balanced equation for the reaction system, including the physical states of each species. From this the equilibrium expression for calculating K_c or K_p is derived.
- the equilibrium concentrations or pressures of each species that occurs in the equilibrium expression, or enough information to determine them. These values are substitued into the equilibrium expression and the value of the equilibrium constant is then calculated.

- Calculating K from Known Equilibrium Amounts
- Calculating K from Initial amounts and One Known Equilibrium Amount
- Calculating K from Known Initial Amounts and the Known Change in Amount of One of the Species

❑ Calculating K from Known Equilibrium Amounts

- Write the equilibrium expression for the reaction.
- Determine the molar concentrations or partial pressures of each species involved.
- Subsititute into the equilibrium expression and solve for K.

Example: Calculate the value of the equilibrium constant, K_c, for the system shown, if 0.1908 moles of CO_2, 0.0908 moles of H_2, 0.0092 moles of CO, and 0.0092 moles of H_2O vapor were present in a 2.00 L reaction vessel were present at equilibrium.

$$CO_2(g) + H_2(g) \leftrightarrows CO(g) + H_2O(g)$$

- Write the equlibrium expression for the reaction system.

$$K_c = \frac{[CO][H_2O]}{[CO_2][H_2]}$$

- Since K_c is being determined, check to see if the given equilibrium amounts are expressed in moles per liter (molarity). In this example they are not; conversion of each is requried.

$[CO_2]$ = 0.1908 mol CO_2/2.00 L = 0.0954 M
$[H_2]$ = 0.0454 M
[CO] = 0.0046 M
$[H_2O]$ = 0.0046 M

- Substitute each concentration into the equilibrium expression and calculate the value of the equilibrium constant.

$$K_c = \frac{[0.0046][0.0046]}{[0.0954][0.0454]} = 0.0049 \text{ or } 4.9 \times 10^{-3}$$

- **Calculating K from Initial Amounts and One Known Equilibrium Amount**

- Write the equilibrium expression for the reaction.
- Determine the molar concentrations or partial pressures of each species involved.
- Determine all equilibrium concentrations or partial pressures using an ICE chart.
- Substitute into the equilibrium expression and solve for K

Example: Initially, a mixture of 0.100 M NO, 0.050 M H_2, 0.100 M H_2O was allowed to reach equilibrium (initially there was no N_2). At equilibrium the concentration of NO was found to be 0.062 M. Determine the value of the equilibrium constant, K_c, for the reaction:

$$2\,NO(g) + 2\,H_2(g) \leftrightarrows N_2(g) + 2\,H_2O(g)$$

- Write the equilibrium expression for the reaction.

$$K_c = \frac{[N_2][H_2O]^2}{[NO]^2[H_2]^2}$$

- Check to see if the amounts are expressed in moles per liter (molarity) since K_c is being . In this example they are.

- Create an ICE chart that expresses the initial concentration, the change in concentration, and the equilibrium concentration for each species in the reaction. From the chart you can determine the changes in the concentrations of each species and the equilibrium concentrations. From the example, we start with the following information.

	NO	H_2	N_2	H_2O
Initial Concentration (M)	0.100	0.0500	0	0.100
Change in Concentration (M)	- 2 x	- 2 x	+ x	+ 2 x
Equilibrium Concentration (M)	0.062			

The change in concentration of the NO was (0.062 M - 0.100M) = - 0.038 M. Thus -2 x = - 0.038 and x = 0.019. Note: the negative sign indicates a decreasing concentration, not a negative concentration. The changes in the other species must agree with the stoichiometry dictated by the balance equation. The hydrogen will also change by - 0.038 M, while the nitrogen will increase by + 0.019 M and the water will increase by + 0.038 M. From these changes we can complete the chart to find the equilibrium concentrations for each species.

	NO	H_2	N_2	H_2O
Initial Concentration (M)	0.100	0.0500	0	0.100
Change in Concentration (M)	- 0.038	- 0.038	+ 0.019	+ 0.038
Equilibrium Concentration (M)	0.062	0.012	0.019	0.138

- Substitute the equilibrium concentrations into the equilibrium expression and solve for K_c.

$$K_c = \frac{[0.019][0.138]^2}{[0.062]^2[0.012]^2} = 650 \text{ or } 6.5 \times 10^2$$

- **Calculating K from Known Initial Amounts and the Known Change in Amount of One of the Species**
- Write the equilibrium expression for the reaction.
- Determine the molar concentrations or partial pressures of each species involved.
- Determine all equilibrium concentrations or partial pressures using an ICE chart.
- Substitute into the equilibrium expression and solve for K.

Example: A flask is charged with 3.00 atm of dinitrogen tetroxide gas and 2.00 atm of nitrogen dioxide gas at 25^{o}C and allowed to reach equilibrium. It was found that the pressure of the nitrogen dioxide decreased by 0.952 atm. Estimate the value of K_p for this system:

$$N_2O_4(g) \leftrightarrows 2\ NO_2(g)$$

- Write the equilibrium expression to find K_p.

$$K_p = \frac{P^2_{(NO2)}}{P_{(N2O4)}}$$

- Check to see that the given amounts are measured in appropriate pressure units since K_p is to be In this example they are (atmospheres).
- Create an ICE chart and calculate the changes in pressure and equilibrium pressures for each species.

	N_2O_4	NO_2
Initial Pressure (atm)	3.00	2.00
Change in Pressure (atm)	+ 0.476	- 0.952
Equilibrium Pressure (atm)	3.476	1.048

- Substitute the equilibrium pressures into the expression for K_p and solve for K_p.

$$K_p = \frac{(1.048)^2}{(3.476)} = 0.3160$$

❑ CONVERTIONS BETWEEN K_C AND K_P

To convert between K_c to K_p use the following equation which is based on the relationship between molarities and gas pressures.

$$K_p = K_c(RT)^{□n}$$

□n is the difference in the number of **moles of gases** on each side of the balanced equation for the reaction.

Δn = (number of moles of gaseous products - number of moles of gaseous reactants)

- Converting K_c to K_p
- Converting K_p to K_c

Converting K_c to K_p

- Calculate the difference in the number of moles of gases.
- Subsititute □n, R, and T into the equation and solve.

Example: Calculate the value of K_p for the following reaction, at 333 K.

$$PH_3BCl_3(s) \leftrightarrows PH_3(g) + BCl_3(g) \quad K_c = 6.96 \times 10^{-5} \text{ @ } 333\text{ K}$$

- Calculate the difference in the number of moles of gases, □n.

□n = (2 moles of gaseous products - **0 moles of gaseous reactants) = 2**

- Substitute the values into the equation and calculate K_p.

$$\mathbf{K_p = (6.96 \times 10^{-5})[(0.0821)(333)]^2 = 0.052}$$

Note: because we do not choose to use units for K_c and K_p , we cannot cancel units for R and T. However, be careful to use the value of R consistent with the units of pressure used in the problem, and T in Kelvin.

Converting K_p to K_c

- Calculate the change in the number of moles of gases.
- Subsititute □n, R, and T into the equation and solve.

Example: Calculate the value of K_c at 373 K for the following reaction:

$$2\ NO(g) + Br_2(g) \leftrightarrows 2\ NOBr(g) \qquad K_p = 2.40\ @\ 373\ K$$

- Calculate the change in the number of moles of gases, □n.

□n = (2 moles of gaseous products - **3 moles of gaseous reactants) = - 1**

- Substitute the values into the equation and calculate K_c.

$$\mathbf{2.40 = K_c[(0.0821)(373)]^{-1}}$$
$$\mathbf{K_c = 73.5}$$

Note: because we do not choose to use units for K_c and K_p , we cannot cancel units for R and T. However, be careful to use the value of R consistent with the units of pressure used in the problem, and T in Kelvin.

Calculating K for a Reaction
Using Known K's for Other Reactions

- K for a Reversed Reaction
- Reaction Coefficients Multiplied by a Number
- Adding Two or More Equations
- Calculations Incorporating Two or More of These Algebraic Manipulations

K for a Reversed Reaction

The equilibrium expression written for a reaction written in the reverse direction is the reciprocal of the one for the forward reaction.

$$K' = 1/K$$

K' is the constant for the reverse reaction and K is that of the forward reaction.

Example: What is the value of the equilibrium constant for the reaction $2\ NO_2(g) \leftrightarrows N_2O_4(g)$ at 100^o C?

$$N_2O_4(g) \leftrightarrows 2\ NO_2(g) \quad K_c = 0.212\ @\ 100^oC?$$

The desired reaction is the reverse of the reaction for which the K_c is known. The equilibrium expression is the reciprocal of that given.

$$K'_c = 1/K_c = 1/0.212 = 4.72$$

Reaction Coefficients Multiplied by a Number

If the coefficients in a balanced equation are multiplied by a factor, n, the equilibrium expression is raised to the n^{th} power.

$$K' = (K)^n$$

K' is the constant for the reaction multiplied by n and K is the constant of the original reaction.

Adding Two or More Equations

If two or more reactions are added to give another, the equilibrium constant for the reaction is the product of the equilibrium constants of the equations added.

$$K' = K_1 \times K_2 \ \ldots$$

K_1 , K_2, etc. represent the equilibrium constants for reactions being added together, and K' represents the equilibrium constant for the desired reaction.

Example: Calculate the value of K_c for the reaction: $2\ NO(g) + Br_2(g) \leftrightarrows 2\ NOBr\ (g)$ using the following information.

$$2\ NO(g) \leftrightarrows N_2(g) + O_2(g) \qquad K_{c1} = 1 \times 10^{30}$$
$$N_2(g) + Br_2(g) + O_2(g) \leftrightarrows 2\ NOBr(g) \qquad K_{c2} = 2 \times 10^{-27}$$

The two equations can be added to yield the desired equation. The value of K_c for the reaction will be the product of the other two.

$$K'_c = K_{c1} \times K_{c2} = (1 \times 10^{30})(1 \times 10^{-27}) = 2 \times 10^3$$

Calculations Incorporating Two or More of These Algebraic Manipulations

It is possible to combine more than one of these manipulations.

Example: Calculate the value of K_c for the reaction: $2\ N_2O(g) + 3\ O_2(g) \leftrightarrows 2\ N_2O_4(g)$, using the following information.

Equation	Equilibrium Constant
$2\ N_2\ (g) + O_2(g) \leftrightarrows 2\ N_2O(g)$	$K_c = 1.2 \times 10^{-35}$
$N_2O_4(g) \leftrightarrows 2\ NO_2(g)$	$K_c = 4.6 \times 10^{-3}$

� $N_2(g) + O_2(g) \leftrightarrows NO_2(g)$	$K_c = 4.1 \times 10^{-9}$

These three equations can be combined to get the desired reaction.

$$\begin{array}{lcl}
2\,N_2O(g) & \leftrightarrows & \cancel{2\,N_2(g)} + \cancel{O_2(g)} \\
\cancel{4\,NO_2(g)} & \leftrightarrows & 2\,N_2O_4(g) \\
\cancel{2\,N_2(g)} + \overset{3}{\cancel{4}}\,O_2(g) & \leftrightarrows & \cancel{4\,NO_2(g)} \\
\hline
2\,N_2O(g) + 3\ \ O_2(g) & \leftrightarrows & 2\,N_2O_4(g)
\end{array}$$

- Write the first equation backwards. The K for this reaction will be the recipricol of the forward reaction.

$$2\,N_2O(g) \leftrightarrows 2\,N_2(g) + O_2(g) \qquad K_c = 1/(1.2 \times 10^{-35}) = \quad 8.3 \times 10^{34}$$

- Write the second equation backwards and multiply the coefficients by 2. The K for this reaction will be the recipricol of the forward reaction squared.

$$4\,NO_2(g) \leftrightarrows 2\,N_2O_4(g) \qquad K_c = 1/(4.6 \times 10^{-3})^2 = \quad 4.7 \times 10^4$$

- Use the third equation in the forward direction but multiplied by 4. The K for this reaction will be the K of the given reaction raised to the fourth power.

$$2\,N_2(g) + 4\,O_2(g) \leftrightarrows 4\,NO_2(g) \qquad K_c = (4.1 \times 10^{-9})^4 = \quad 2.8 \times 10^{-34}$$

- Check to see that the three equations yield the desired equation when added together. The equilibrium constant for the desired equation will be the product of the constants for the three equations combined.

$$K_c = (8.3 \times 10^{34})(4.7 \times 10^4)(2.8 \times 10^{-34}) = 1.1 \times 10^6$$

❑ CALCULATING THE REACTION QUOTIENT, Q

The expression for the reaction quotient, Q, looks like that used to calculate an equilibrium constant but Q can be calculated for any set of conditions, not just for equilibrium.

Q can be used to determine which direction a reaction will shift to reach equilibrium. If K > Q, a reaction will proceed forward, converting reactants into products. If K < Q, the reaction will proceed in the reverse direction, converting products into reactants. If Q = K then the system is already at equilibrium.

In order to determine Q we need to know:

- the equation for the reaction, including the physical states,
- the quantities of each species (molarities and/or pressures), all measured at the same moment in time.

To calculate Q:

- Write the expression for the reaction quotient.
- Find the molar concentrations or partial pressures of each species involved.
- Subsitute values into the expression and solve.

Example: 0.035 moles of SO_2, 0.500 moles of SO_2Cl_2, and 0.080 moles of Cl_2 are combined in an evacuated 5.00 L flask and heated to 100^oC. What is Q before the reaction begins? Which direction will the reaction proceed in order to establish equilibrium?

$$SO_2Cl_2(g) \leftrightarrows SO_2(g) + Cl_2(g) \qquad K_c = 0.078 \text{ at } 100^oC$$

- Write the expression to find the reaction quotient, Q.

$$Q_c = \frac{[SO_2][Cl_2]}{[SO_2Cl_2]}$$

- Since K_c is given, the amounts must be expressed as moles per liter (molarity). The amounts are in moles so a conversion is required.

0.500 mole SO_2Cl_2/5.00 L = 0.100 M SO_2Cl_2

0.035 mole SO_2/5.00 L = 0.070 M SO_2

0.080 mole Cl_2/5.00 L = 0.016 M Cl_2

- Substitute the values in to the expression and solve for Q.

$$Q_c = \frac{(0.070)(0.016)}{(0.100)} = 0.011$$

- Compare the answer to the value for the equilibrium constant and predict the shift.

0.078 (K) > 0.011 (Q)

Since K >Q, the reaction will proceed in the forward direction in order to increase the concentrations of both SO_2 and Cl_2 and decrease that of SO_2Cl_2 until Q = K.

- **Determining Equilibrium Quantities from Initial Quantities and K**

To find the equilibrium quantities of each species from the initial quantities we must know:

- the balanced equation for the reaction
- the equilibrium expression for the reaction
- the value for the equilibrium constant
- the initial quantities of each species, either as molarities, or partial pressures
- the direction the reaction will proceed in order to establish equilibrium

Once these have been determined, we can solve for the equilibrium concentrations using the following steps:

- Write the equilibrium expression for the reaction.
- Check to see that the quantities are expressed in the same units as used in the equilibrium constant.
- Determine the direction the reaction will shift. Calculate Q if direction of shift is uncertain.
- Make an ICE chart and determine the equilibrium quantities in terms of a single unknown change.
- Substitute into the equilibrium expression and solve for the change.
- Calculate the equilibrium quantity for each species from the initial quantity and the change.
- Check your work.
- Determining Equilibrium Concentrations
- Determining Equilibrium Pressures

Determining Equilibrium Concentrations

Example: 0.050 mol of H_2 and 0.050 mol of Br_2 are placed in an evacuated 5.0 L flask and heated to 700 K. What is the concentration of each species in the flask when equilibrium has been established? The equation for the reaction is as follows:

$$H_2(g) + Br_2(g) \leftrightarrows 2\,HBr(g) \qquad K_c = 64 \text{ @ } 700\text{ K}$$

- Write the equilibrium expression for the reaction.

$$K_c = \frac{[HBr]^2}{[H_2][Br_2]} = 64$$

- Since K_c is used in this problem, check to see if the given quantities are in moles per liter (molarity). In this example they are not. A conversion is required.

$$[H_2] = 0.050 \text{ mole } H_2/5.0\text{ L} = 0.010\text{ M}$$
$$[Br_2] = 0.010\text{ M}$$
$$[HBr] = 0\text{ M}$$

- The only direction that this reaction can proceed is forward due to the fact that initially there are only H_2 and Br_2 in the flask. The reverse reaction cannot begin to occur until some HBr is formed.

- Make an ICE chart with "x" representing the change in the concentration of the H_2 (or Br_2) as the system moves towards equilibrium. All of the other changes are expressed in terms of x.

	H_2	Br_2	HBr
Initial Concentration (M)	0.010	0.010	0
Change in Concentration (M)	- x	- x	+ 2 x
Equilibrium Concentration (M)	0.010 - x	0.010 - x	0 + 2 x

- Substitute the expressions for the equilibrium concentrations into the equilibrium expression and solve for "x".

$$64 = \frac{(2x)^2}{(0.010 - x)(0.010 - x)} = \frac{(2x)^2}{(0.010 - x)^2}$$

x = 0.008 M

- Calculate the equilibrium concentration for each species from the initial concentrations and the changes.

$[H_2] = [Br_2] = 0.010 - x = 0.010 - 0.008 = 0.002$ M for each
$[HBr] = 2x = 2(0.008) = 0.016$ M

- Check your answer by substituting the equilibrium concentrations into the equilibrium expression and see if the result is the same as the equilibrium constant.

$$\frac{(0.016)^2}{(0.002)(0.002)} = 64$$

❑ **Determining Equilibrium Pressures**

Example: 1.000 atm of SO_3, 0.150 atm of SO_2, 0.200 atm of NO_2, and 2.000 atm of NO at 460^{o}C was allowed to reach equilibrium. What is the equilibrium pressure of each gas present in the flask?

$$SO_2(g) + NO_2(g) \leftrightarrows NO(g) + SO_3(g) \quad K_p = 85.0 \text{ @ } 460^oC$$

- Write the equilibrium expression for the reaction.

$$K_p = \frac{P_{(NO)}P_{(SO3)}}{P_{(SO2)}P_{(NO2)}} = 85.0$$

- Since we are using K_p, check to see if the given quantities are in appropriate pressure units (atmospheres). In this example they are, so no conversion is required.
- Calculate the value of the reaction quotient, Q, to determine the direction the reaction will proceed to reach equilibrium.

$$Q = \frac{(1.500)(2.000)}{(0.150)(0.200)} = 100$$

$K_p < Q$ so the reaction will proceed in the reverse direction.

- Make an ICE chart. Let "x" represnt the change in the pressure of the NO. Since the reaction proceeds in the reverse direction, the NO and SO_3 will decrease and the SO_2 and NO_2 will increase as equilibrium is established.

SO_2 NO_2

http://www.chem.purdue.edu/gchelp/howtosolveit/howtosolveit.html#Equilibrium

http://home.sbc.edu.hk/~chem/Supp%20Ex%20solution%20guideline/SuppEx_4B_E.pdf.