ICE charts/diagram/table

ICE diagrams

When a reversible reaction takes place a state of equilibrium will be reached where the concentrations remain the same. In this case the equilibrium constant can be used to set up an equation describing the state of the reaction.

For example for the following reaction A + B ↔ C+ D will have an equilibrium equation like

$$keq = \frac{[C][D]}{[A][B]}$$

*The task now is to determine the concentrations at equilibrium given *some* *__initial__* *or* *__final__* *condition*. This is the purpose of the ICE Diagram. *

The **ICE Diagram**

The trick is to set up the above equation remembering that any change in concentration must be consistent with the chemical reaction that is the heart of the matter. The ICE Diagram is a table in which the columns represent the different molecules. The different rows are described below.

- First row for the **Initial concentrations (I)**: Place the initial concentrations for each molecule on the first row.

- Second row for the **Change in concentrations (C)**: Here create a variable designating the change in concentrations due to the reaction. Here we assume a net direction for the reaction and give the assumed reactants a negative sign and the product a positive sign. For example in the above reaction (assuming that the reaction flows from right to left) the **change in concentration of A and B can be called -x** and the change in **concentration for C and D is +x**. In the case that coefficients exits indicating that more than one of a particular

molecule is involved, the change row must reflect this. Consider the following

reaction:

$$2A + B \leftrightarrow 3C + D$$

We can let x represent the change in concentration of B or D.

$$\Delta A = -2x, \Delta B = -x, \Delta C = +3x, \Delta D = +x$$

- Third row for the **Equilibrium concentration (E)**: This is just the initial concentrations plus the change in concentrations.

You use the equilibrium concentrations in the equation involving the equilibrium constant

Example:
A mixture of 1.0 mole carbon dioxide and 1.0 mole carbon monoxide are contained in a 1 liter vessel. Later 2.0 moles of water vapor is then introduced into the vessel. The following reversible reaction takes place

$$CO + H_2O \leftrightarrow CO_2 + H_2$$

This reaction has an equilibrium constant of 0.64. How many moles of the different molecules will be present after equilibrium is obtained?

Since there is initially no hydrogen gas in the vessel the reaction must begin going from the left to the right. So let the right side be the reactants and the left the product. So now consider the rows of the ICE table.

- Since the vessel has a volume of 1 L, the number of moles must equal the molarity. So the concentration of CO and CO_2 is 1.0 m, the H_2O is 2.0 m and the H_2 has zero molarity.
- Since all the coefficients are 1 the change is simple. Assuming that the left is the reactants.

$$\Delta CO = -x, \Delta H_2O = -x, \Delta CO_2 = +x, \Delta H_2 = +x$$

- The equilibrium is just the sum of the above.

So now put all this together into an ICE table.

R	CO	H_2O	CO_2	H_2
I (initial)	1.0 M	2.0 M	1.0 M	Ø
C (change)	-x	-x	+x	+x
E (Equilibrium)	1.0 - x	2.0 - x	1.0 + x	x

So now feed the last row into our equilibrium equation

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

$$0.64=\frac{(1.0+x)(x)}{(1.0-x)(2.0-x)}$$

Now to solve for the unknown variable. We can cross-multiply to eliminate the fractions then foil.

$$0.64(1.0-x)(2.0-x)=(1.0+x)(x)$$

$$1.28-1.92x+0.64x^2=x+x^2$$

Move all the variables to one side

$$0=0.36x^2+2.92x-1.28$$

We can solve this using the quadratic equation, graphing etc. Our two solutions are x = -8.5, 0.42 m. The first solution cannot be physically realistic as it would mean that hydrogen would end up with a negative concentration. So the latter number must be the desired solution. Putting our value for x into the last row of our ICE table gives the final concentrations as well as the number of moles.

Molecule	Moles
CO	0.58
H_2O	1.58
CO_2	1.42
H_2	0.42

Note: It usually is not necessary to use the equilibrium equation if you are given the beginning conditions and some information as to the final condition.

Ex 1

1. 3.00 moles of N_2 gas and 1.00 mole of H_2 gas are combined in a 1 L reaction vessel. At equilibrium 0.663 moles of H_2 remain. What are the resulting concentrations?

$$N_2 + 3H_2 \Leftrightarrow 2NH_3$$

Ex 2

$$2NH_{3(g)} \rightleftharpoons N_{2(g)} + 3H_{2(g)}$$

When 4.0 mol of NH_3(g) is introduced into a 2.0L rigid container and heated to a particul temperature, the amount of ammonia changes to 2.0 mol. Determine the equilibrium concentration of the other two entities.

Ex 3

a)

For the system, if we start with 0.100mol/L of CO_2 and H_2, what are the concentrations of the reactants and products at equilibrium given that K_{eq} = 0.64 at 900K?

$$CO_2 + H_2 \leftrightarrow CO + H_2O$$

b)

At 650°C, the reaction below has a K_{eq} value of 0.771. If 2.00 mol of both hydrogen and carbon dioxide are placed in a 4.00 L container and allowed to react, what will be the equilibrium concentrations of all four gases?

Ex 1

1. 3.00 moles of N_2 gas and 1.00 mole of H_2 gas are combined in a 1 L reaction vessel. At equilibrium 0.663 moles of H_2 remain. What are the resulting concentrations?

$$N_2 + 3H_2 \Leftrightarrow 2NH_3$$

Ex 2

$$2NH_{3(g)} \rightleftharpoons N_{2(g)} + 3H_{2(g)}$$

When 4.0 mol of $NH_3(g)$ is introduced into a 2.0L rigid container and heated to a particul temperature, the amount of ammonia changes to 2.0 mol. Determine the equilibrium concentration of the other two entities.

Ex 3

For the system, if we start with 0.010 mol/L of H_2 and I_2 and 0.096 mol/L o HI, what are their concentrations at equilibrium given that Keq= 0.016?

Ex 1

1. 3.00 moles of N_2 gas and 1.00 mole of H_2 gas are combined in a 1 L reaction vessel. At equilibrium 0.663 moles of H_2 remain. What are the resulting concentrations?

$$N_2 + 3H_2 \Leftrightarrow 2NH_3$$

R	N_2	$+ 3H_2 \rightleftharpoons$	$2NH_3$
I	3.0	1.0	0
C	-x	-3x	+2x
E	3.0-x	0.663	2x

$$1.0-3x = 0.663$$

$$X = 0.112$$

$3.0-x = 3.0-0.112$ $[N_2] = 2.89$ mol/L

$2x = 2(0.112)$ $[NH_3] = 0.224$ mol/L

N_2

Ex 2

$2NH_{3(g)} \rightleftharpoons N_{2(g)} + 3H_{2(g)}$

When 4.0 mol of $NH_3(g)$ is introduced into a 2.0L rigid container and heated to a particular temperature, the amount of ammonia changes to 2.0 mol. Determine the equilibrium concentration of the other two entities.

$NH_{3(g)}$ initial =4.0 mol/2.0L = 2 M

$NH_{3(g)}$ equilibrium 2.0 mol/2.0L = 1 M

	$2NH_{3(g)} \rightleftharpoons$	$N_{2(g)}$ +	$3H_{2(g)}$
I	2.0	0	0
C	-2x	+x	+3x
E	1.0	x	3x

2.0 - 2x = 1.0

x $[N_2]$= 0.50 mol/L

3x $[H_2]$= 1.5 mol/L

Ex 3

For the system, if we start with 0.100mol/L of CO_2 and H_2, what are the concentrations of the reactants and products at equilibrium given that $K_{eq} = 0.64$ at 900K?

$$CO_2 \quad + \quad H_2 \quad \leftrightarrow \quad CO \quad + \quad H_2O$$

	CO_2 +	H_2 $\leftrightarrow$	CO +	H_2O
I	0.100	0.100	0	0
C	- x	- x	+ x	+ x
E	0.100 - x	0.100 - x	+ x	+ x

$$K_{eq} = \frac{[CO][H_2O]}{[H_2][CO_2]} = 0.64$$

$$K_{eq} = \frac{(x)(x)}{(0.100 - x)(0.100 - x)} = 0.64 \quad \text{then} \quad \sqrt{\frac{x^2}{(0.100 - x)^2}} = \sqrt{0.64}$$

$$\frac{x}{0.100 - x} = 0.80$$

$$x = 0.080 - 0.80x$$

$$1.80x = 0.080 \quad \text{and} \quad x = 0.044$$

$$\therefore\ [CO]_{eq} = [H_2O]_{eq} = 0.044\ M \text{ and } [CO_2]_{eq} = [H_2]_{eq} = 0.100 - 0.044 = 0.056\ M$$

At 650°C, the reaction below has a K_{eq} value of 0.771. If 2.00 mol of both hydrogen and carbon dioxide are placed in a 4.00 L container and allowed to react, what will be the equilibrium concentrations of all four gases?

$$CO_2 + H_2 \leftrightarrow CO + H_2O$$

	H_2	+ CO_2	$\leftrightarrow$ CO	+ H_2O
I	0.500	0.500	0	0
C	- x	- x	+ x	+ x
E	0.500 - x	0.500 - x	+ x	+ x

$$K_{eq} = \frac{[CO][H_2O]}{[CO_2][H_2]} = 0.771$$

$$K_{eq} = \frac{(x)(x)}{(0.500 - x)(0.500 - x)} = 0.771 \quad \text{then} \quad \sqrt{\frac{x^2}{(0.500 - x)^2}} = \sqrt{0.771}$$

$$\frac{x}{0.500 - x} = 0.878$$

$$x = 0.439 - 0.878x \quad \text{then} \quad x = 0.234$$

$$\therefore\ [CO]_{eq} = 0.260\,M,\ [H_2O]_{eq} = 0.234\ M \text{ and } [H_2]_{eq} = [CO_2]_{eq} = 0.500 - 0.234 = 0.266\ M$$

Ex 3

For the system, if we start with 0.010 mol/L of H_2 and I_2 and 0.096 mol/L of HI, what are their concentrations at equilibrium given that Keq= 0.016?

	$2\,HI \rightleftharpoons$	H_2 +	I_2
I	0.096	0.010	0.010
C	-2x	+x	+x
E	0.096 - 2x	0.010 + x	0.010 + x

$$K_{eq} = \frac{[H_2][I_2]}{[HI]^2}$$

s

$$\sqrt{0.016} = \sqrt{\frac{[0.010+x]^2}{[0.096-2x]^2}}$$

$$(0.096-2x)\,0.126 = \frac{[0.010+x}{0.096-2x} \quad x$$

$$0.096-2x(0.126) = 0.010 + x$$

$$1.252x = 0.002$$

$$x = 0.0016$$

$x = 0.0016$

$[HI] = 0.096 - 2x = 0.093$ mol\L

$[H_2]$ & $[I_2] = 0.010 + x = 0.012$ mol/L

Ex 3

For the system, if we start with 0.010 mol/L of H_2 and I_2 and 0.096 mol/L of HI, what are their concentrations at equilibrium given that Keq= 0.016?

	$2\,HI \rightleftharpoons$	H_2 +	I_2
I	0.096	0.010	0.010
C	-2x	+x	+x
E	0.096 - 2x	0.010 + x	0.010 + x

$$K_{eq} = \frac{[H_2][I_2]}{[HI]^2}$$

$$0.016 = \frac{[0.010+x][0.010+x]}{[0.096-2x]^2}$$

$$\sqrt{0.016} = \sqrt{\frac{(0.010+x)^2}{(0.096-2x)^2}}$$

$$0.126 = \frac{0.010+x}{0.096-2x}$$

$$0.126(0.096-2x) = 0.010 + x$$

$$0.0121 - 0.252x = 0.010 + x$$

$$0.0121 - 0.010 = 0.252x + x$$

$$\frac{0.0021}{1.252} = \frac{1.252x}{1.252}$$

$$x = 0.0167$$

Homework

Questions 1-4

Keq Extra Problems assignment 16 questions.docx

Quiz Section 18.1 & 18.2

Quiz Friday

Correction

1. Considering the following equilibrium:

$$2AB_{3(g)} \leftrightarrow A_{2(g)} + 3B_{2(g)}$$

If 0.87 moles of AB_3 are injected into a 5.0L container at 25ºC, at equilibrium the final $[A_2]$ is found to be 0.070M. (Hint: make a table and use it to answer the questions below).

$$A_2 + B \rightleftharpoons 2C$$

I	0	0	1.5
C	$+x$	$+x$	$-2x$
E	0.30	0.30	$1.5-2x$

18.1

Objectives

- Describe how to express the rate of a chemical reaction
- Identify four factors that influence the rate of a chemical reaction

Vocabulary

- rate
- collision theory
- activation energy
- activated complex
- transition state
- inhibitor

18.2

Objectives

- Describe how the amounts of reactants and products change in a chemical system at equilibrium
- Identify three stresses that can change the equilibrium position of a chemical system
- Explain what the value of K_{eq} indicates about the position of equilibrium

Vocabulary

- reversible reaction
- chemical equilibrium
- equilibrium position
- Le Châtelier's principle
- equilibrium constant (K_{eq})

Key Equation

- $K_{eq} = \frac{[C]^c \times [D]^d}{[A]^a \times [B]^b}$

  When $aA + bB \rightleftharpoons cC + dD$

18.1

- Four factors that affect the rate of reaction
- rate- measure of speed/interval of time
- key terms

18.2

- reversible reactions
- Le Chatelier's Principle- factors affecting equilibrium
  > **Concentration** -
    - increased conc shifts to opposite side
    - decreased conc shifts to same side
  > **Heat**
    - increase in temperature shifts to side without heat
    - decrease in temp shifts to the side with heat
  > **Pressure** -
    - increase in pressure shifts to side with least moles of gas
    - decrease in pressure shifts to side with most moles of gas
- $K_{eq} = \frac{[C]^c[D]^d}{[A]^a[B]^b}$
- $[A]^a$ is a concentration value in mol/1.0 L or molarity(M)
- $K_{eq} > 1$~ products favored
- $K_{eq} < 1$~ reactants favored
- ICE tables

11.

$$CO + H_2O \rightleftharpoons CO_2 + H_2$$

	CO	H_2O	CO_2	H_2
I	0.01	0.01	0.01	0.01
C	$-x$	$-x$	$-x$	$-x$
E	$0.01-x$	$0.01-x$	$0.01-x$	$0.01-x$

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

$$\sqrt{0.400} = \sqrt{\frac{(0.01-x)^2}{(0.01-x)^2}}$$

$$0.632 = \frac{0.01-x}{0.01-x}$$

$$0.632(0.01-x) = 0.01 - x$$

$$-0.632x + x = 0.01 - 6.32\times10^{-3}$$

$$0.368x = 3.68\times10^{-3}$$

$$x = 0.01$$

Quiz 18.1 & 18.2

Section review answers SKMBT_50117110115160.pdf

SKMBT_50117110115161.pdf

Practice quiz answers

SKMBT_50117110115162.pdf

review practice for 181 & 182 quiz.tst

Chem Help today 12:30 and 3:15 - 4:00

__1__ measure the speed of any change that occurs within a time interval. Collision theory states that particles __2__ when they collide, provided that they have enough __3__.

The rate at which a chemical reaction occurs is determined by an __4__ energy barrier. The activation energy is the __5__ energy that reactants must have to be converted to __6__. The higher the activation energy barrier, the __7__ the reaction. Chemists help reactants overcome the activation barrier in a number of ways. Two effective methods are to increase the __8__ at which the reaction is done or use a __9__. Rates of reaction can also be increased by __10__ the concentration of reactants.

1. Rates
2. react
3. Kinetic energy
4. activation
5. minimum
6. products
7. slower
8. temperature
9. catalyst
10. increasing

Part B True-False

Classify each of these statements as always true, AT; sometimes true, ST; or never true, NT.

ST **11.** An increase in temperature will increase the rate of a reaction.

Name ____________ Date ____________ Class ____________

NT **12.** A catalyst is considered as a reactant in a chemical reaction.

AT **13.** The speed of a reaction can be increased by increasing reactant concentration or decreasing particle size.

AT **14.** An enzyme is a biological catalyst.

Column A	Column B
15. rate	a. synonym for an activated complex
16. collision theory	b. speed of a change that occurs over time
17. activation energy	c. substance that interferes with the action of a catalyst
18. transition state	d. Particles can react to form products when they collide, provided they have enough kinetic energy.
19. activated complex	e. an unstable arrangement of atoms that forms momentarily at the peak of the activation energy barrier
20. inhibitor	f. minimum energy that particles must have in order to react

Part D Questions and Problems

Answer the following question and solve the following problem in the space provided.

21. An ice machine can produce 120 kg of ice in 24 hours. Express the rate of ice production in kg/h.

$$\frac{120\ \text{kg}}{24\ \text{h}} = 5.0\ \text{kg/h}$$

Part A Completion

Use this completion exercise to check your understanding of the concepts and terms that are introduced in this section. Each blank can be completed with a term, short phrase, or number.

In principle, all reactions are __1__. That is, reactants go to __2__ in the __3__ direction, and products go to __4__ in the __5__ direction.

The point at which the rate of conversion of __6__ to __7__ and vice versa is equal is the __8__ position. The __9__ of a reversible reaction, K_{eq}, is useful for determining the position of equilibrium. It is essentially a measure of the __10__ of products to reactants at equilibrium. The direction of change in the position of equilibrium may be predicted by applying __11__ principle.

1. reversible
2. products
3. forward
4. reactants
5. reverse
6. reactants
7. products
8. equilibrium
9. equilibrium constant
10. ratio
11. LeChatelier's

Part B True-False

Classify each of these statements as always true, AT; sometimes true, ST; or never true, NT.

NT 12. The concentrations of reactants and products in a system at dynamic equilibrium are always changing.

ST 13. A change in the pressure on a system can cause a shift in the equilibrium position.

NT 14. For a chemical equilibrium to be established, the chemical reaction must be irreversible.

AT 15. The K_{eq} for a certain reaction was 2×10^{-7}. For this reaction at equilibrium, the concentration of the reactants is greater than the concentration of the products.

$$K_{eq} = \frac{[\text{products}]}{[\text{reactants}]}$$

$= \frac{10}{1}$

or

$= \frac{1}{10}$

Part C Matching

Match each description in Column B to the correct term in Column A.

Column A	Column B
d 16. reversible reaction	a. state of balance in which forward and reverse reactions take place at the same rate
a 17. chemical equilibrium	b. relative concentrations of reactants and products of a reaction that has reached equilibrium
b 18. equilibrium position	c. When stress is applied to a system at equilibrium, the system changes to relieve the stress.
c 19. Le Châtelier's principle	d. reaction in which conversion of reactants to products and products to reactants occur simultaneously
e 20. equilibrium constant	e. ratio of product concentrations to reactant concentrations with each raised to a power given by the number of moles of the substance in the balanced equation

Part D Problem

Solve the following problem in the space provided. Show your work.

21. $2SO_3(g) \rightarrow 2SO_2(g) + O_2(g)$

Calculate K_{eq} for this reaction if the equilibrium concentrations are:
$[SO_2] = 0.42M$, $[O_2] = 0.21M$, $[SO_3] = 0.072M$

$$K_{eq} = \frac{[0.42\,m]^2 \times [0.21\,m]}{[0.072\,m]^2}$$

$= 7.145 = 7.1 > 1$, so favours products

MC

1. B
2.
3.
4
5
6
7
8
9
10

11. • $K_{eq} = \frac{[C]^c \times [D]^d}{[A]^a \times [B]^b}$

$$K_{eq} = \frac{[C]^2}{[A]^3 [B]^2}$$

12. $K_{eq} = \dfrac{[NO]^2[Cl_2]}{[NClO]^2}$

$K_{eq} = \dfrac{[6.4]^2[0.99]}{[1.6]^2} = 7.8$

7.8

13. $PCl_3 + Cl_2 \rightleftharpoons PCl_5$

	PCl_3	Cl_2	PCl_5
I	0	0	1.5
C	$+x$	$+x$	$-x$
E	x	x	1.2

$1.5 - x = 1.2$

$x = 0.30$

$$Keq = \frac{[PCl_5]}{[PCl_3][Cl_2]} = \frac{1.2}{(0.3)^2}$$

$Keq = 13$

14. $H_2 + I_2 \rightleftharpoons 2HI$

	H_2	I_2	$2HI$
I	0	0	$3.4 \div 2 = 1.7$
C	$+x$	$+x$	$-2x$
E	x	x	$1.7-2x$

$$K_{eq} = \frac{[HI]^2}{[H_2][I_2]}$$

$$\sqrt{49} = \sqrt{\frac{[1.7-2x]^2}{x^2}}$$

$$7 = \frac{1.7-2x}{x} \quad x \cancel{x}$$

$$7x = 1.7-2x$$

$$7x+2x = 1.7$$

$$\frac{9x}{9} = \frac{1.7}{9}$$

$$x = 0.19$$

[H2] =0.19

[I2] = 0.19

[HI] = 1.7-2(x)

1.7- 2(0.19)
= 1.32

15. $3A_{(g)} + B_{(s)} \rightleftharpoons C_{(s)} + 2D_{(g)}$

$$K_{eq} = \frac{[D]^2}{[A]^3} = 1.4 \times 10^{-4} = \frac{[D]^2}{[0.24]^3}$$

$$(1.4 \times 10^{-4})\,[0.24]^3 = [D]^2$$

$$D = 1.4 \times 10^{-3} \text{ mol/L}$$

16. a - shifts left

b. shifts right

c. shifts right

d. shifts right

You use the equilibrium concentrations in the equation involving the equilibrium constant

Example:
A mixture of 1.0 mole carbon dioxide and 1.0 mole carbon monoxide are contained in a 1 liter vessel. Later 2.0 moles of water vapor is then introduced into the vessel. The following reversible reaction takes place

$$CO + H_2O \leftrightarrow CO_2 + H_2$$

This reaction has an equilibrium constant of 0.64. How many moles of the different molecules will be present after equilibrium is obtained?

Since there is initially no hydrogen gas in the vessel the reaction must begin going from the left to the right. So let the right side be the reactants and the left the product. So now consider the rows of the ICE table.

- Since the vessel has a volume of 1 L, the number of moles must equal the molarity. So the concentration of CO and CO_2 is 1.0 m, the H_2O is 2.0 m and the H_2 has zero molarity.
- Since all the coefficients are 1 the change is simple. Assuming that the left is the reactants.

  $$\Delta CO = -x,\ \Delta H_2O = -x,\ \Delta CO_2 = +x,\ \Delta H_2 = +x$$
- The equilibrium is just the sum of the above.

So now put all this together into an ICE table.

	CO	H_2O	CO_2	H_2
I (initial)	1.0 M	2.0 M	1.0 M	Ø
C (change)	-x	-x	+x	+x
E (Equilibrium)	1.0 - x	2.0 - x	1.0 + x	x

So now feed the last row into our equilibrium equation

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

$$0.64=\frac{(1.0+x)(x)}{(1.0-x)(2.0-x)}$$

Now to solve for the unknown variable. We can cross-multiply to eliminate the fractions then foil.

$$0.64(1.0-x)(2.0-x)=(1.0+x)(x)$$

$$1.28-1.92x+0.64x^2=x+x^2$$

Move all the variables to one side

$$0 = 0.36x^2 + 2.92x - 1.28$$

We can solve this using the quadratic equation, graphing etc. Our two solutions are x = -8.5, 0.42 m. The first solution cannot be physically realistic as it would mean that hydrogen would end up with a negative concentration. So the latter number must be the desired solution. Putting our value for x into the last row of our ICE table gives the final concentrations as well as the number of moles.

Molecule	Moles
CO	0.58
H_2O	1.58
CO_2	1.42
H_2	0.42

Note: It usually is not necessary to use the equilibrium equation if you are given the beginning conditions and some information as to the final condition.

Attachments

Keq Extra Problems assignment 16 questions.docx

SKMBT_50117110115160.pdf

SKMBT_50117110115161.pdf

SKMBT_50117110115162.pdf

review practice for 181 & 182 quiz.tst