

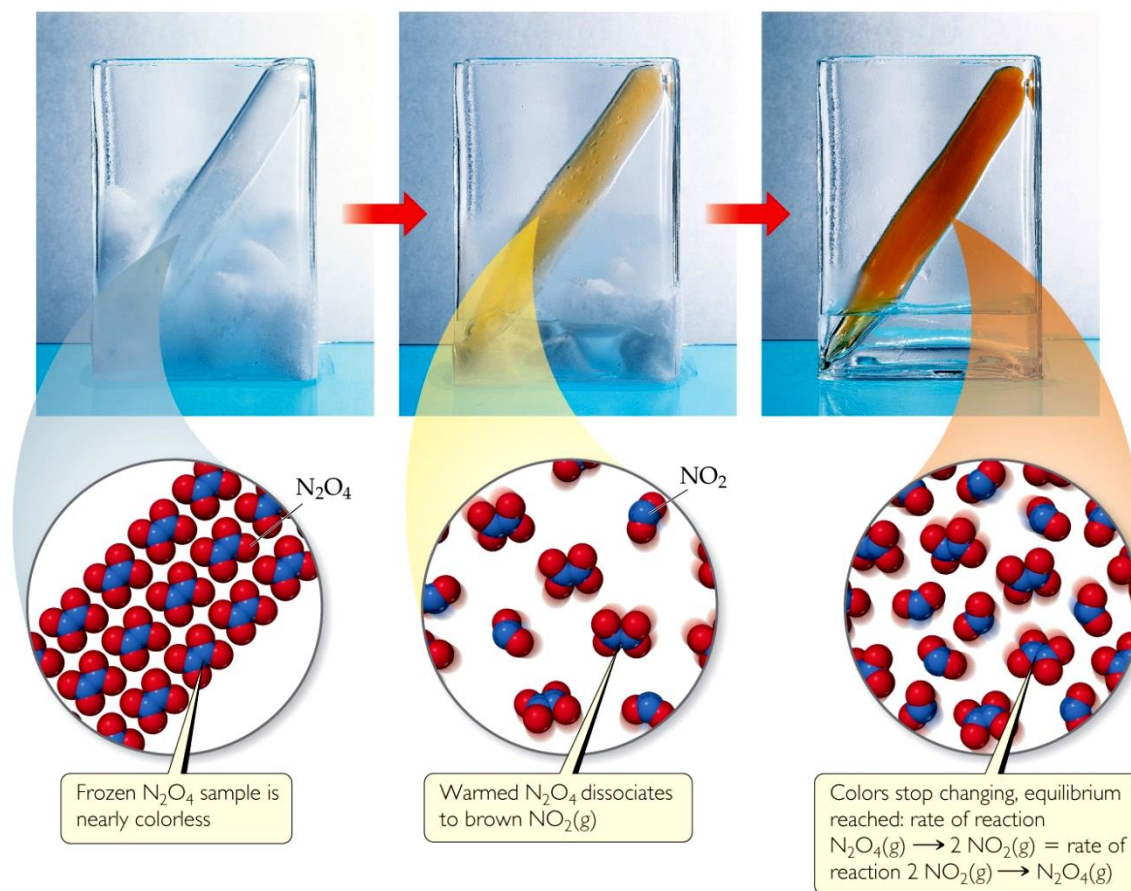
Chapter 15

Chemical Equilibrium

By Zhen-Yu Wu

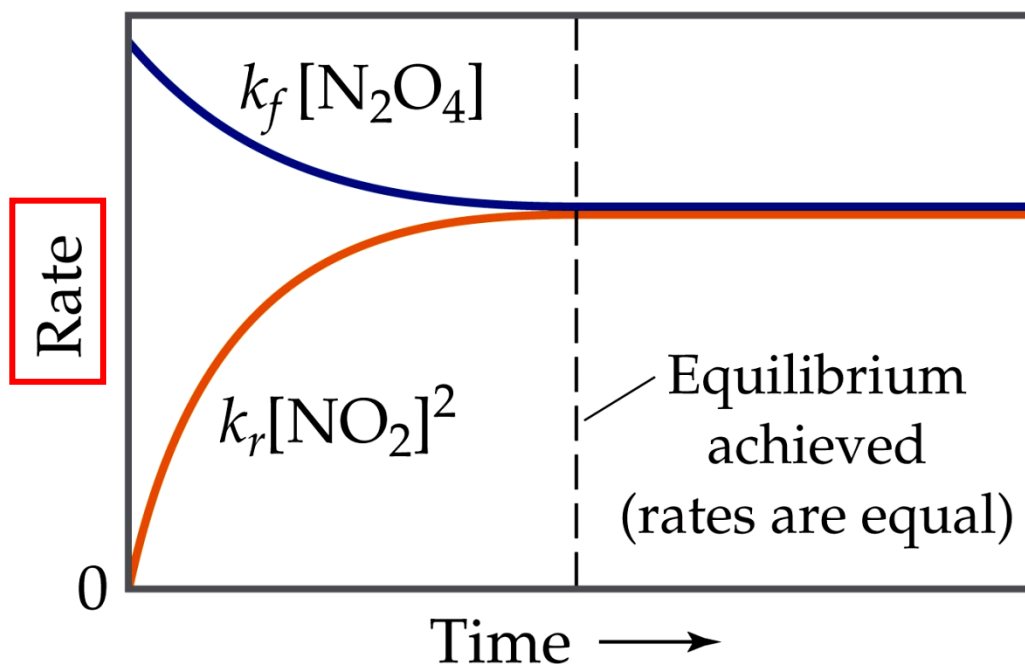
➤ The Concept of Equilibrium (平衡)

❑ **Chemical equilibrium** occurs when a reaction and its reverse (逆向) reaction proceed at the same rate



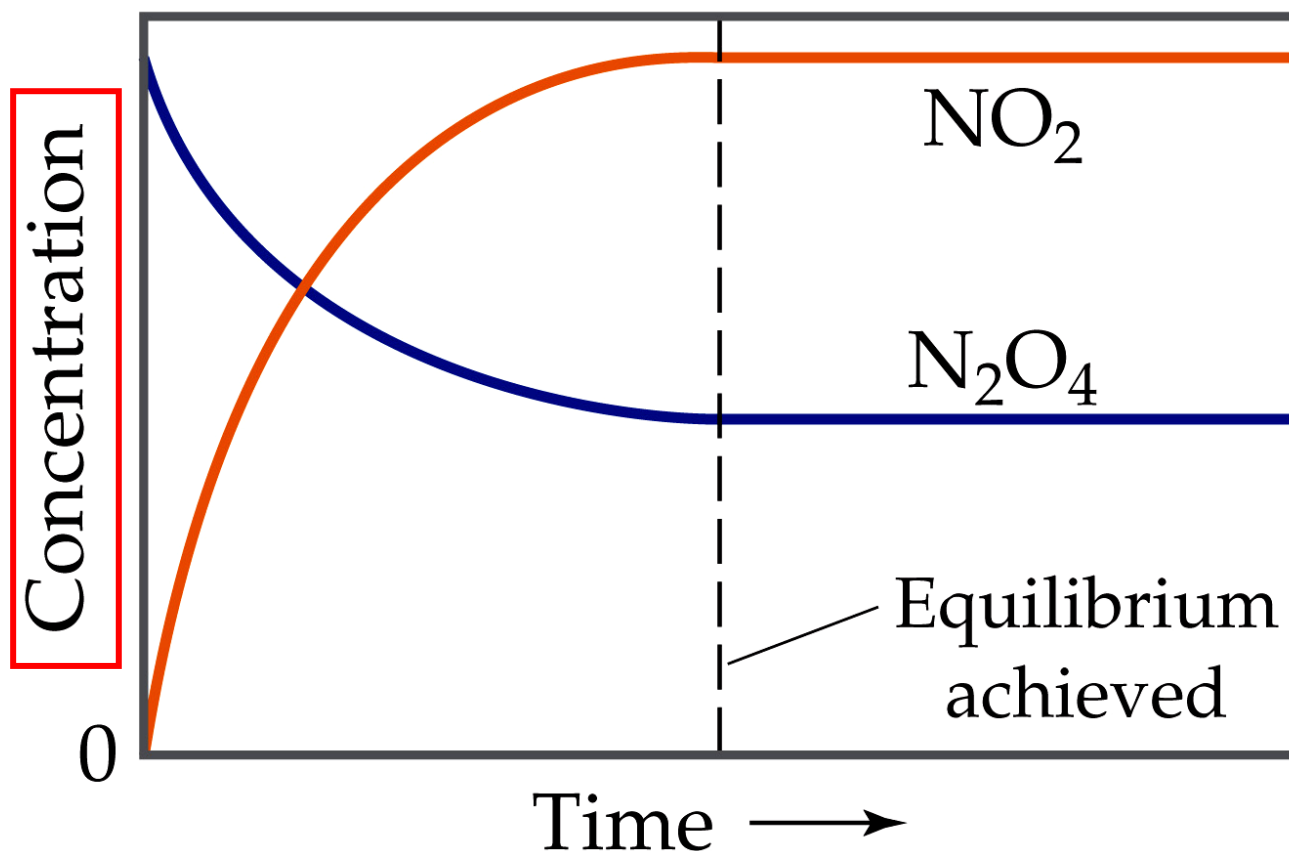
➤ The Concept of Equilibrium (平衡)

- ❑ As a system approaches (接近) equilibrium, both the forward and reverse reactions are occurring.
- ❑ At equilibrium, the forward and reverse reactions are proceeding ***at the same rate***.



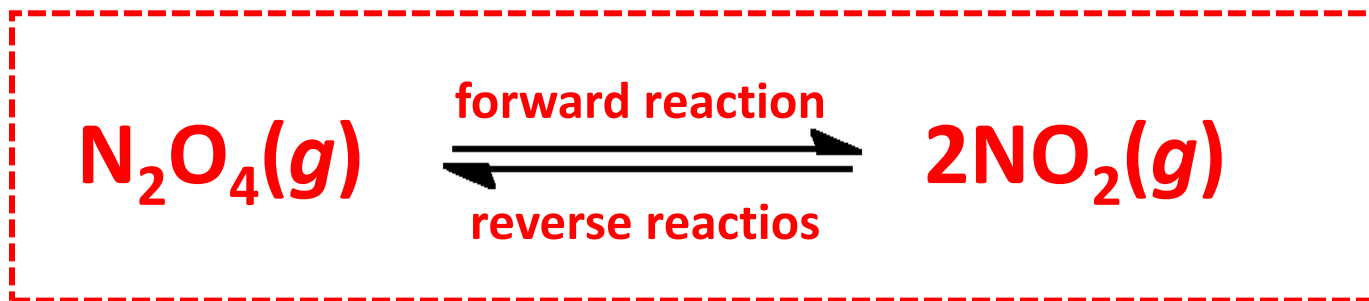
➤ A System at Equilibrium

- Once equilibrium is achieved (达到), the *amount* of each reactant and product remains constant.

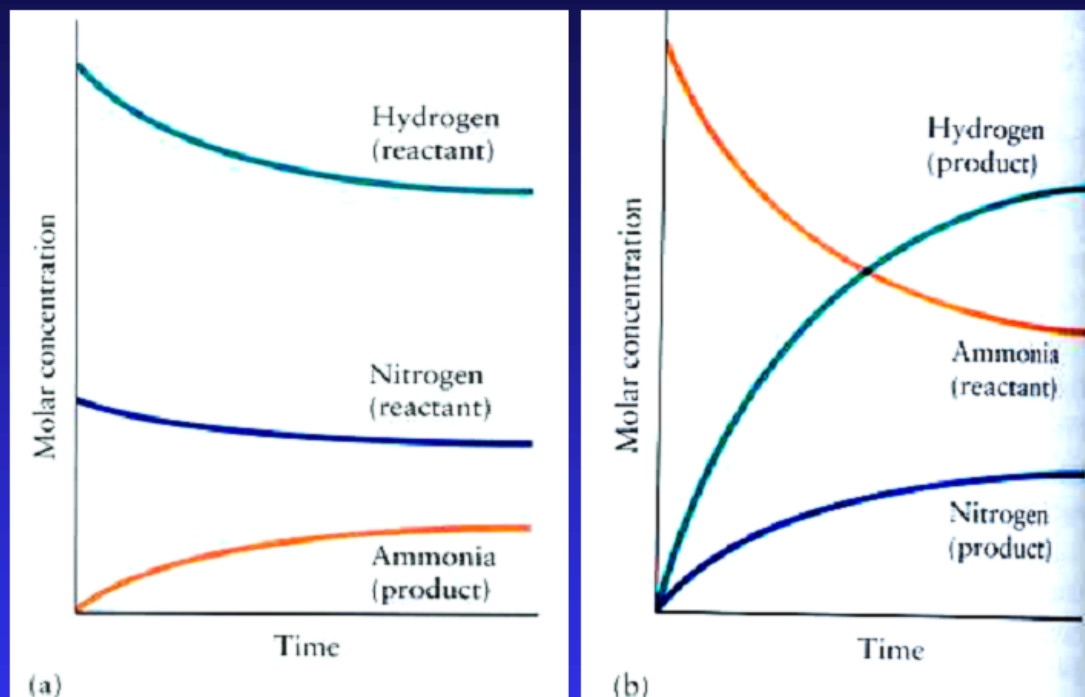
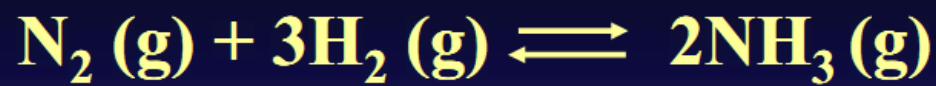


➤ Depicting Equilibrium

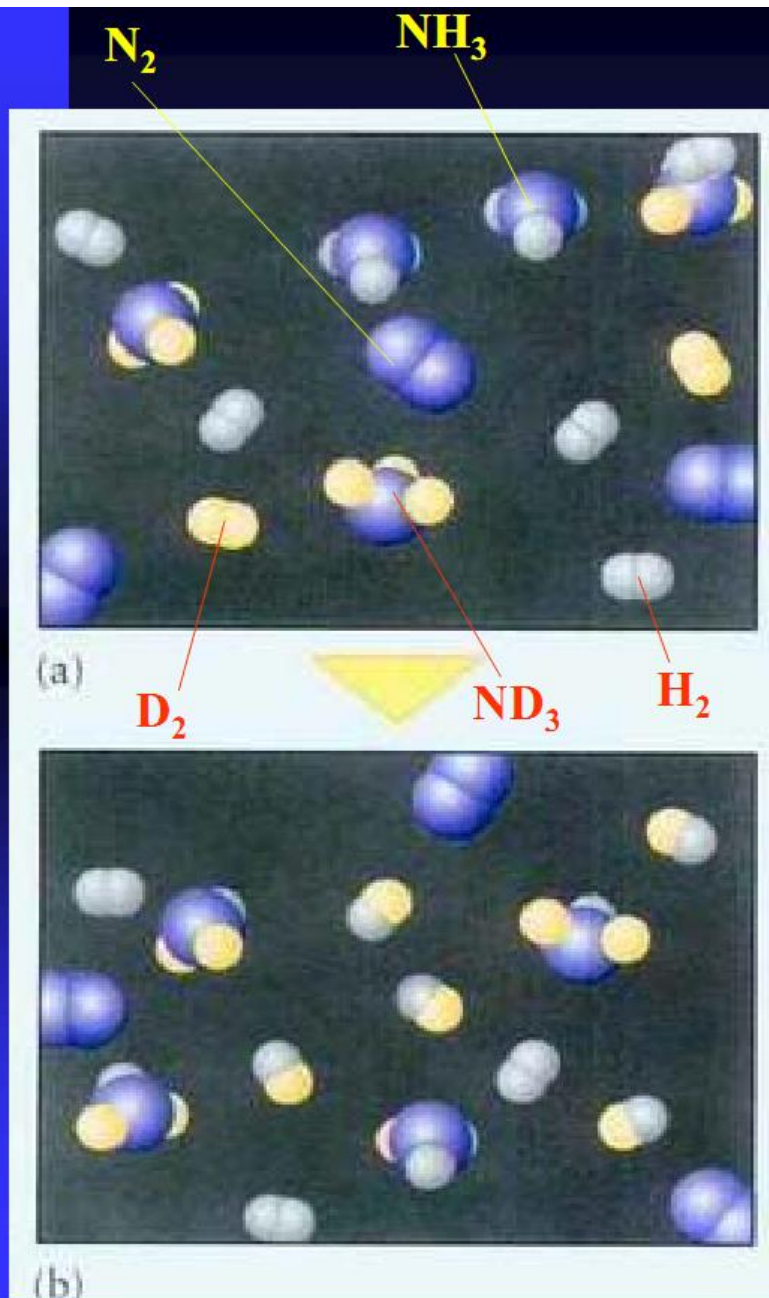
- Since, in a system at equilibrium, both the forward and reverse reactions are being carried out, we write its equation with a double arrow:



- 因为一般化学反应都是可逆进行的，即正向和反向反应同时进行。当反应进行到一定程度，正向反应的速率和逆向反应速率逐渐相等，反应物和生成物的浓度就不再发生变化，这种表面静止的状态就叫做“平衡状态”。处在平衡状态的物质浓度称为“平衡浓度”。



- (a) In the synthesis of ammonia, the concentrations of N_2 , H_2 decrease with time and that of NH_3 increase until they finally settle into values corresponding to a mixture in which all three are present and there is no further net change.
- (b) If the experiment is repeated with pure ammonia, it decomposes, and the composition settles down into a mixture of NH_3 , H_2 , and N_2 .



动态平衡的实验证据

In an experiment showing that equilibrium is dynamic.

- (a) A reaction mixture in which N_2 , D_2 , and ND_3 have reached equilibrium is mixed with one with the same concentrations of N_2 , H_2 , and NH_3 .
- (b) After some time, the concentrations of N_2 , hydrogen and ammonia are found to be the same, but the D atoms are distributed among the hydrogen and ammonia molecules.

➤ The Equilibrium Constant

□ Forward reaction:



□ Rate law:

$$\text{Rate} = k_f[\text{N}_2\text{O}_4] \quad (k_f = \text{rate constant})$$

□ Reverse reaction:



□ Rate law:

$$\text{Rate} = k_r[\text{NO}_2]^2 \quad (k_r = \text{rate constant})$$

➤ The Equilibrium Constant

□ Therefore, at equilibrium

$$\text{Rate}_f = \text{Rate}_r$$

$$k_f[\text{N}_2\text{O}_4] = k_r[\text{NO}_2]^2$$

□ Rewriting this, it becomes

$$\frac{k_f}{k_r} = \frac{[\text{NO}_2]^2}{[\text{N}_2\text{O}_4]}$$

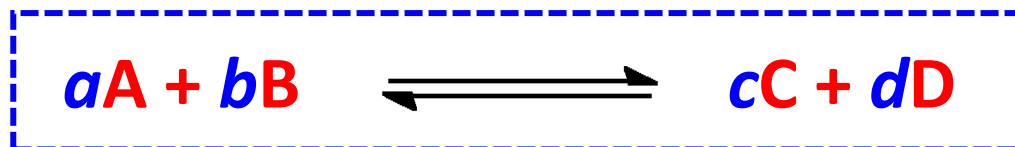
➤ The Equilibrium Constant

- The ratio (比) of the rate constants is a constant at that **temperature**, and it is called equilibrium constant (K_{eq})

$$K_{eq} = \frac{k_f}{k_r} = \frac{[NO_2]^2}{[N_2O_4]}$$

➤ The Equilibrium Constant

- Consider the generalized reaction



- The equilibrium expression for this reaction would be

c for concentration expressed in molarity

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

➤ The Equilibrium Constant

- Since pressure is proportional to concentration for gases in a closed system, the equilibrium expression can also be written

$$K_p = \frac{(P_C)^c (P_D)^d}{(P_A)^a (P_B)^b}$$

➤ Relationship Between K_c and K_p

□ From the ideal-gas law we know that

$$PV = nRT$$

□ Rearranging it, we get

$$P = \frac{n}{V} RT$$

➤ Relationship Between K_c and K_p

$$P_X = \frac{n_X}{V} RT = [X] RT$$

recall

$$K_p = \frac{(P_C)^c (P_D)^d}{(P_A)^a (P_B)^b}$$

$$K_p = \frac{([C]RT)^c ([D]RT)^d}{([A]RT)^a ([B]RT)^b}$$

$$K_p = K_c (RT)^{\Delta n}$$

Where $\Delta n = (c + d) - (a + b)$

(moles of gaseous product) – (moles of gaseous reactant)

(二) 平衡常数

是表明化学反应限度的一种特征值。



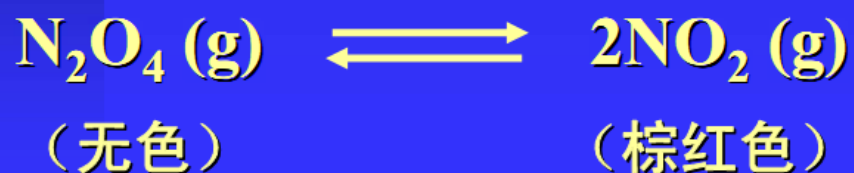
在温度 T 时，平衡浓度 $[\text{A}]$, $[\text{B}]$, $[\text{C}]$, $[\text{D}]$ 之间有：

$$\frac{[\text{C}]^p[\text{D}]^q}{[\text{A}]^m[\text{B}]^n} = K$$

其中 K 是常数，叫作该反应在温度 T 的平衡常数。这个常数可由实验直接测定，称为经验平衡常数或实验平衡常数 K 。

N₂O₄-NO₂体系的平衡浓度 (373K)

试验次序		起始浓度 $\text{mol} \cdot \text{dm}^{-3}$	浓度变化 $\text{mol} \cdot \text{dm}^{-3}$	平衡浓度 $\text{mol} \cdot \text{dm}^{-3}$	$\frac{[\text{NO}_2]^2}{[\text{N}_2\text{O}_4]}$
1	N ₂ O ₄	0.100	-0.060	0.040	0.36
	NO ₂	0.000	+0.120	0.120	
2	N ₂ O ₄	0.000	+0.014	0.014	0.37
	NO ₂	0.100	-0.028	0.072	
3	N ₂ O ₄	0.100	-0.030	0.070	0.36
	NO ₂	0.100	+0.060	0.160	



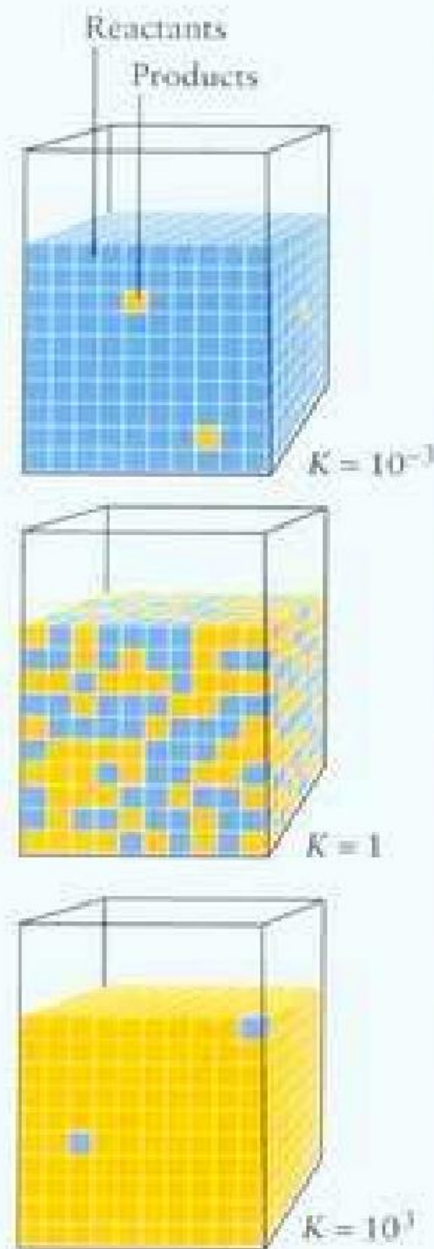
- 1) 起始浓度不同，平衡浓度也不同。
- 2) 只要温度一定，平衡常数即一定。

● 平衡常数的物理意义:

平衡常数 K 值的大小表明反应进行的程度(也叫反应的限度)。 K 值越大,表明反应进行越完全。

由实验测定了物质的转化率,就可求出平衡常数。知道了平衡常数,又可以计算其它起始状态的物质的转化率。一个反应在某一定温度下只有一个特征的平衡常数,但反应中物质的转化率可以不同。

The size of the equilibrium constant indicates whether the reactants or the products are favored. Note that reactants are favored when K is small, products are favored when K is large, and reactants and products are in equal abundance when $K = 1$.



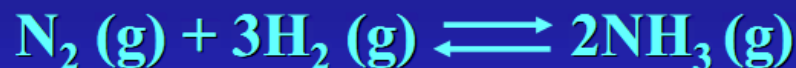
● 书写和应用平衡常数时的注意事项

- 1) 平衡常数表示式要与化学方程式相对应，并注明温度。平衡体系的化学方程式可以有不同的写法， K 值的表示也随之不同。此时尽管具体数值有所差别，但其实际含义是相同的。



2) 平衡常数值依浓度表示方法的不同而异。当浓度用 $\text{mol}\cdot\text{dm}^{-3}$ 时(通常情况), K 可用 K_c 表示。

气相反应的转化率常用分压或摩尔分数表示, 其平衡常数可分别用 K_p 或 K_x 表示。例如,



$$K_c = \frac{[\text{NH}_3]^2}{[\text{N}_2][\text{H}_2]^3} \quad K_p = \frac{p_{\text{NH}_3}^2}{p_{\text{N}_2} \cdot p_{\text{H}_2}^3} \quad K_x = \frac{x_{\text{NH}_3}^2}{x_{\text{N}_2} \cdot x_{\text{H}_2}^3}$$

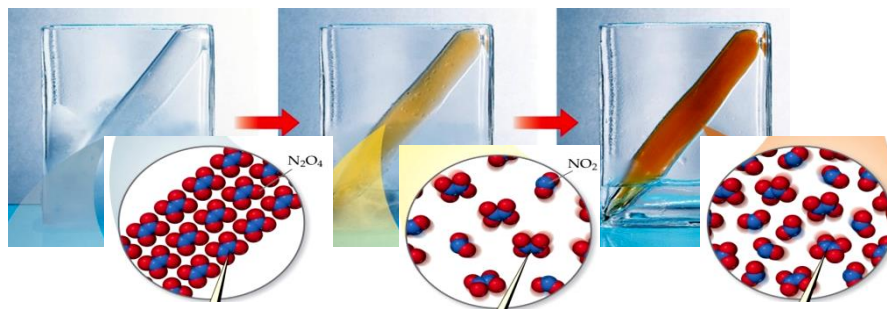
当各种气体都符合理想气体定律时, 三种 K 之间的关系为:

$$pV = nRT \quad p = n/V RT = cRT \quad p_{\text{N}_2} = p \cdot x_{\text{N}_2}$$

$$K_p = K_c(RT)^{\Delta n} \quad K_p = K_x p^{\Delta n}$$

➤ Equilibrium Can Be Reached from Either Direction

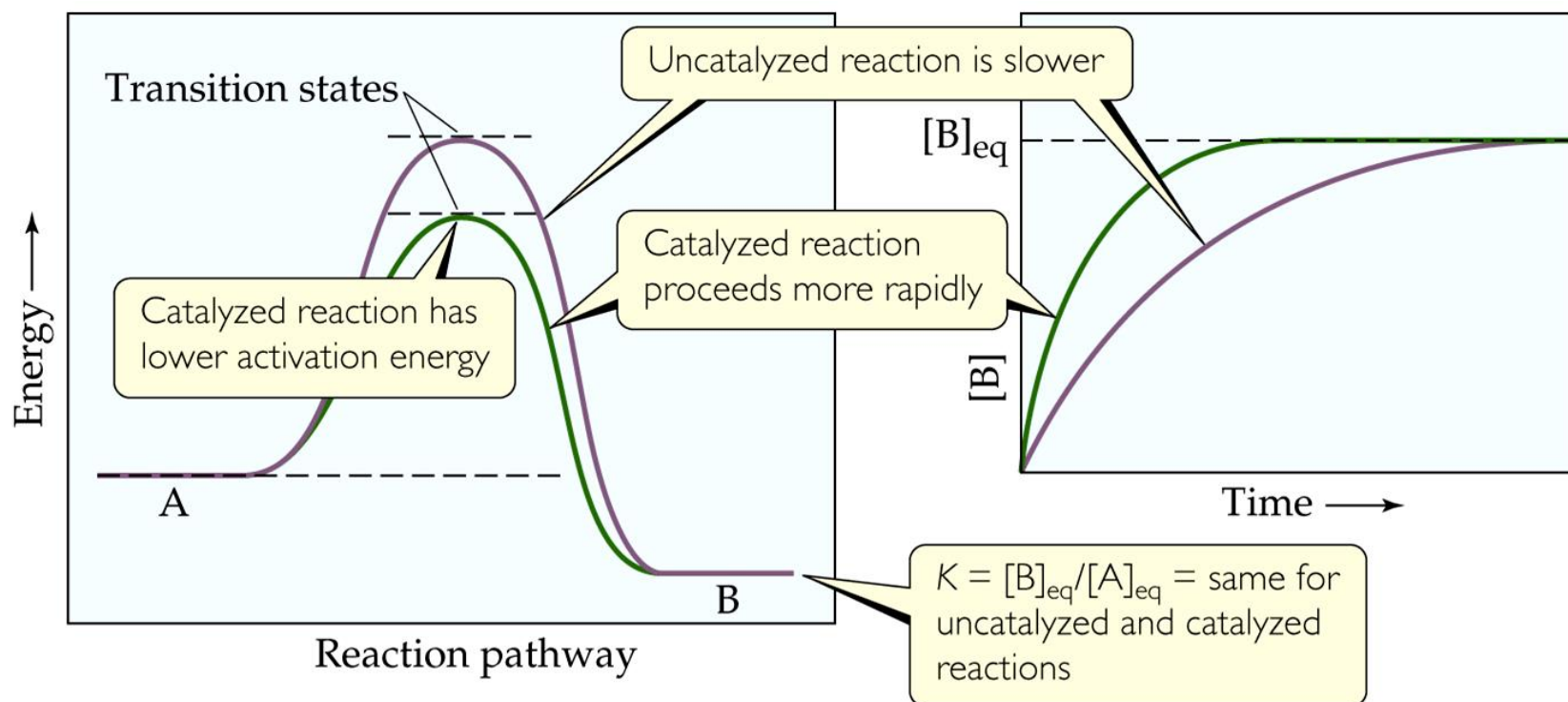
- ❑ As you can see, the ratio of $[\text{NO}_2]^2$ to $[\text{N}_2\text{O}_4]$ remains constant at this temperature no matter what the initial concentrations of NO_2 and N_2O_4 are.



Experiment	Initial $[\text{N}_2\text{O}_4]$ (M)	Initial $[\text{NO}_2]$ (M)	Equilibrium $[\text{N}_2\text{O}_4]$ (M)	Equilibrium $[\text{NO}_2]$ (M)	K_c
1	0.0	0.0200	0.00140	0.0172	0.211
2	0.0	0.0300	0.00280	0.0243	0.211
3	0.0	0.0400	0.00452	0.0310	0.213
4	0.0200	0.0	0.00452	0.0310	0.213

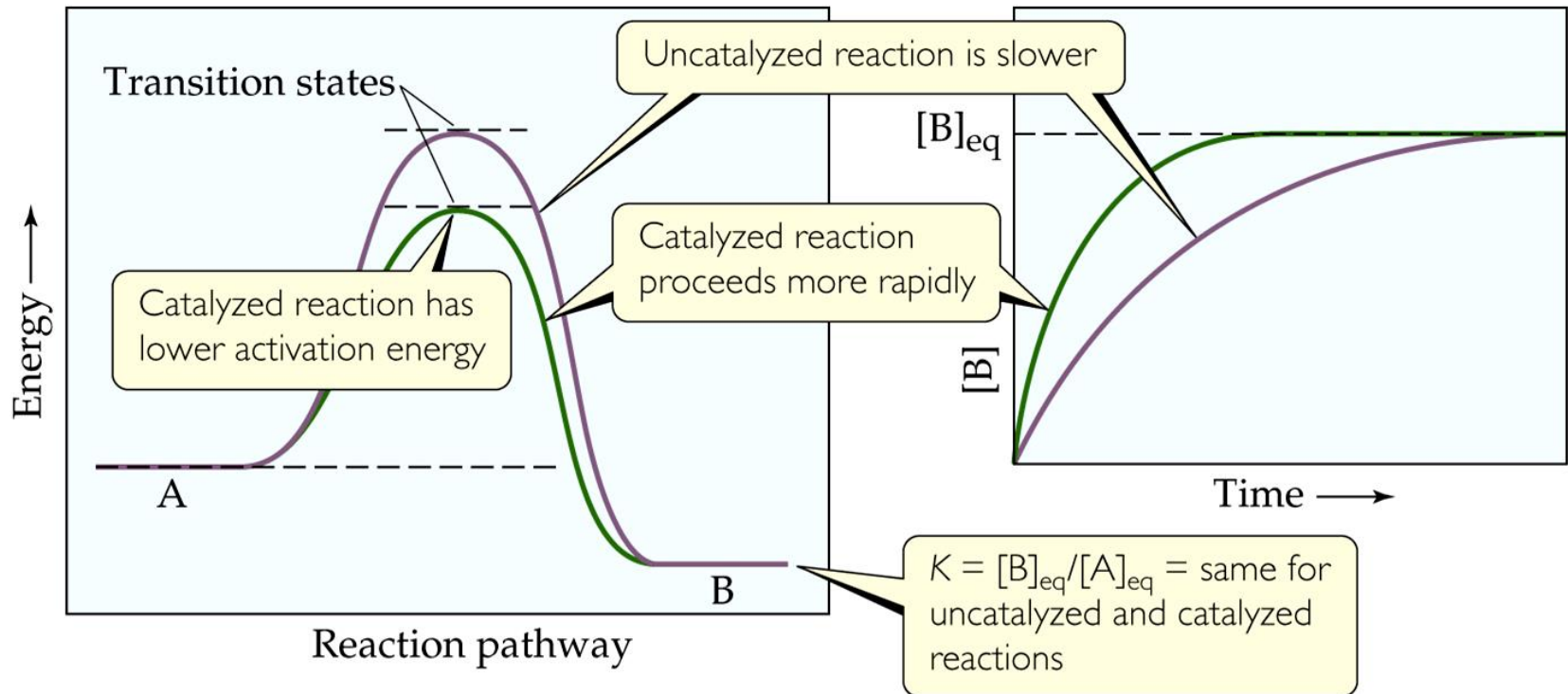
➤ Catalysts

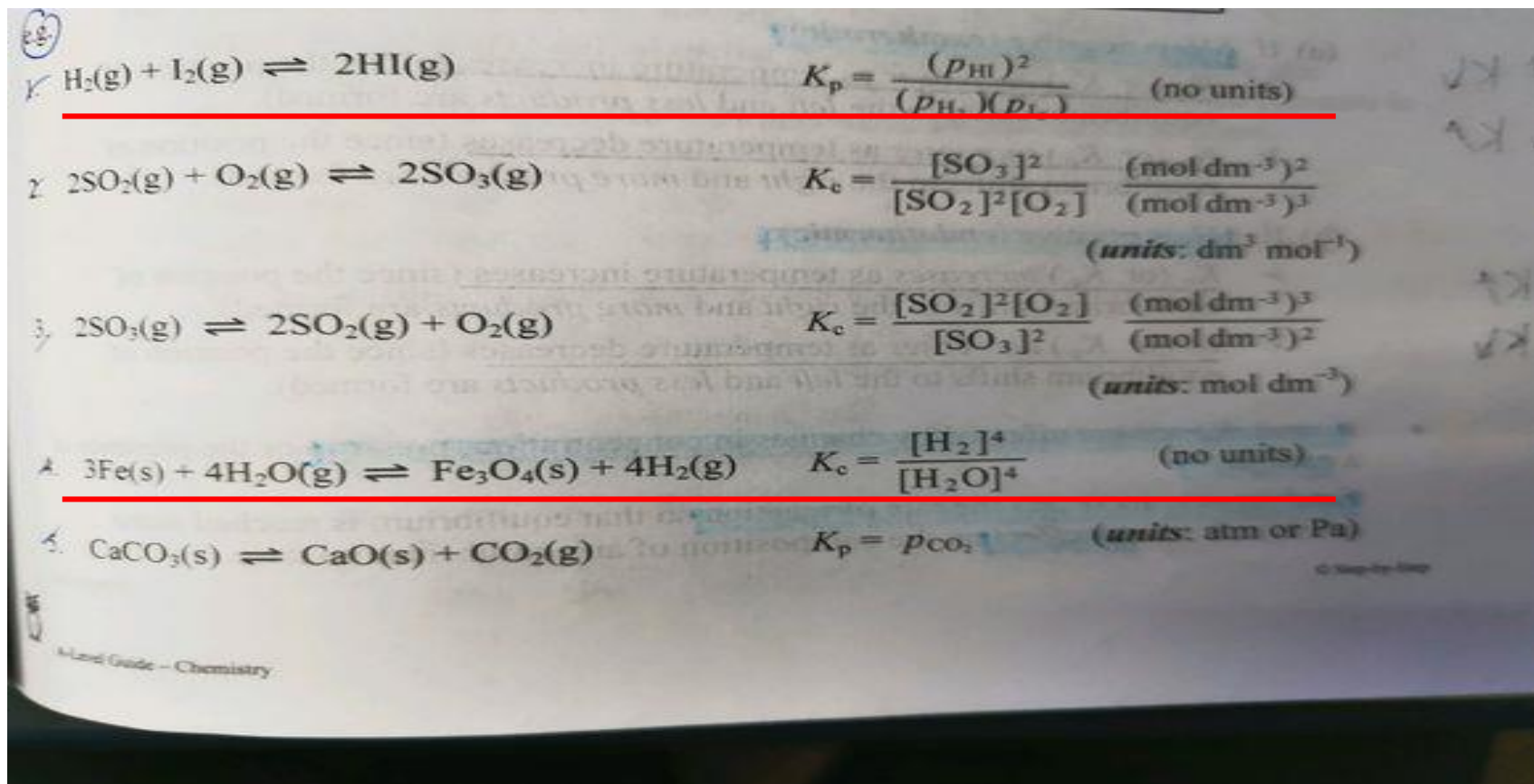
- ❑ Catalysts increase the rate of both the forward *and* reverse reactions.



➤ Catalysts

- ❑ When one uses a catalyst, equilibrium is achieved faster, but the equilibrium composition remains unaltered.





对于反应物计量系数之和等于生成物计量系数之和的反应，其**经验平衡常数**是无量纲的纯数，与压力、浓度所用的单位无关，而且也等于**标准平衡常数**之值。对于反应物计量系数之和不等于生成物计量系数之和的反应，则其经验平衡常数是有量纲的量，其数值就与压力、浓度所用的单位有关。只有当压力、浓度的单位与热力学数据表中对应标准态的单位相同时，所计算的**经验平衡常数**数值才能与**标准平衡常数**数值相同。**从本质上讲，它确是没有量纲的量，而且二者是统一的。**中学教材中涉及的化学平衡常数是经验平衡常数，故在高考题中所考的平衡常数是有单位的。

➤ Equilibrium Constants and Units

- Equilibrium constants derived from thermodynamic measurements are defined in terms of *activities* rather than concentrations or partial pressures.
- **Activity** (活度 symbol a) is a measure of the “effective concentration” of a species in a mixture

$$a = \gamma \cdot c / c_o$$

Where

γ = activity coefficient,

c = concentration;

c_o = reference concentration (1 M)

➤ Equilibrium Constants and Units

$$a = \gamma \cdot p / p_o$$

Where

c = concentration;

p_o = reference pressure (1 atm)

- Both activity and the activity coefficient are dimensionless (无量纲no unit), therefore equilibrium constants are reported without unit
- In simplicity, $\gamma = 1$; $a = c$ and $a = p$

3) 平衡常数不写量纲。

4) 对于非理想溶液，应以活度 α 代替浓度 c 。



$$\frac{\alpha_{\text{C}}^p \cdot \alpha_{\text{D}}^q}{\alpha_{\text{A}}^m \cdot \alpha_{\text{B}}^n} = K$$

If the concentration of N_2O_4 in an equilibrium mixture is 0.00140 M , what is its activity? (Assume the solution is ideal.)

A. 0.00140 M

☒ B. 0.00140 (no units)

C. 0.00140 atm

D. Requires reference concentration to calculate ratio

Proper definition of equilibrium constant involves ratio of activities, not concentrations, and activities are dimensionless by definition.

Ex.:

$$K = \frac{a_{\text{H}^+} a_{\text{A}^-}}{a_{\text{HA}}}$$

Activity may be expressed as a product of an activity coefficient and the relative concentration, which is dimensionless as well, because it is calculated as molar concentration divided by standard concentration, which is conventionally chosen to be

$$c_0 = 1 \text{ mol/l}$$

.

Ex.:

$$a_{\text{H}^+} = \gamma_{\text{H}^+} [\text{H}^+] = \gamma_{\text{H}^+} c_{\text{H}^+} / c_0$$

In textbook examples we usually simplify calculations by setting activity coefficients to unity, thus equilibrium constant is expressed in relative concentrations

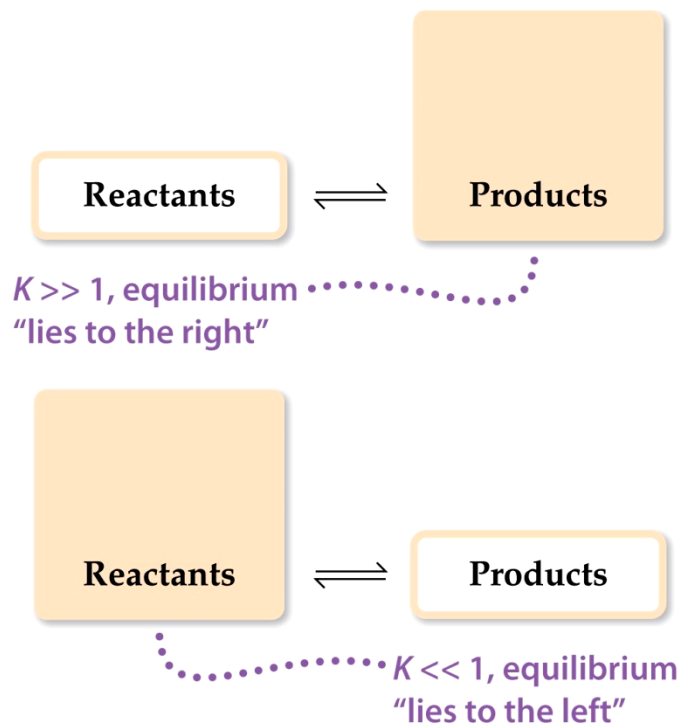
$$K = \frac{[\text{H}^+][\text{A}^-]}{[\text{HA}]}$$

At this step people (even specialists and authors of textbooks) often forget, that concentrations are still relative = dimensionless.

This is the contemporary view - you might find different and less consistent approach in historical books.

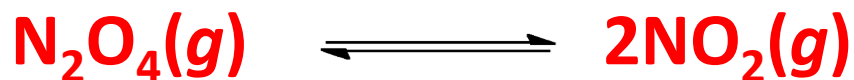
➤ What Does the Value of K Mean?

- ❑ If $K \gg 1$, the reaction is *product-favored*; product predominates (主导) at equilibrium.
- ❑ If $K \ll 1$, the reaction is *reactant-favored*; reactant predominates at equilibrium.

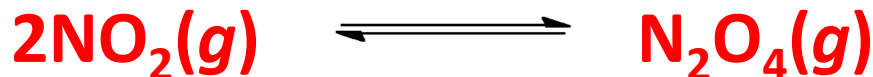


➤ Manipulating Equilibrium Constants

- ❑ The equilibrium constant of a reaction in the reverse reaction is the reciprocal (倒数) of the equilibrium constant of the forward reaction:



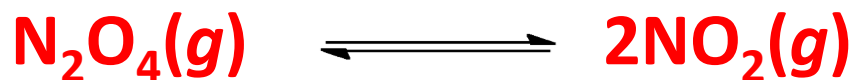
$$K_c = \frac{[\text{NO}_2]^2}{[\text{N}_2\text{O}_4]} = 0.212 \text{ at } 100^\circ\text{C}$$



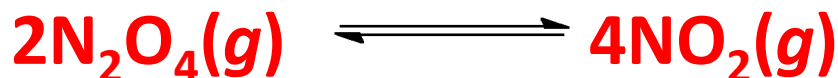
$$K_c = \frac{[\text{N}_2\text{O}_4]}{[\text{NO}_2]^2} = 4.72 \text{ at } 100^\circ\text{C}$$

➤ Manipulating Equilibrium Constants

- The equilibrium constant of a reaction that has been multiplied by a number is the equilibrium constant raised to a power that is equal to that number:



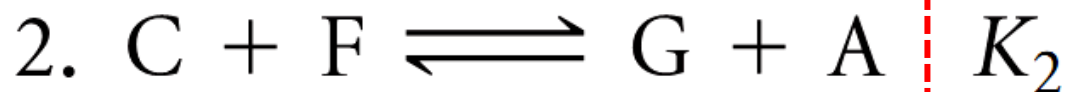
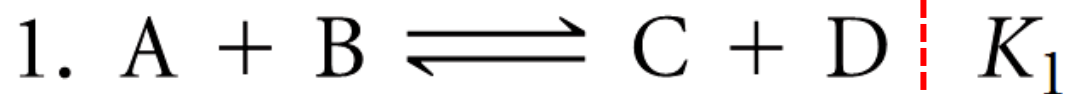
$$K_c = \frac{[\text{NO}_2]^2}{[\text{N}_2\text{O}_4]} = 0.212 \text{ at } 100^\circ\text{C}$$



$$K_c = \frac{[\text{NO}_2]^4}{[\text{N}_2\text{O}_4]^2} = (0.212)^2 \text{ at } 100^\circ\text{C}$$

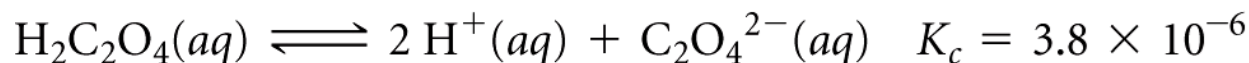
➤ Manipulating Equilibrium Constants

- ❑ The equilibrium constant for a net (淨) reaction made up of two or more steps is the product of the equilibrium constants for the individual steps.

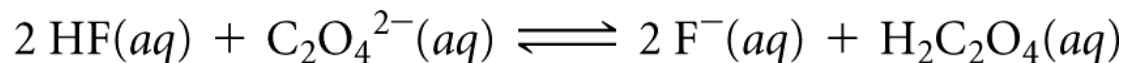


Exercise Combining Equilibrium Expressions

Given the reactions $\text{HF}(aq) \rightleftharpoons \text{H}^+(aq) + \text{F}^-(aq)$ $K_c = 6.8 \times 10^{-4}$



determine the value of K_c for the reaction

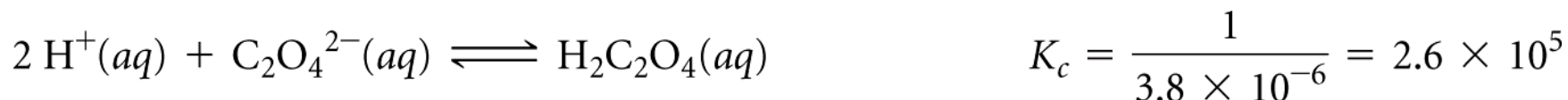


Solution

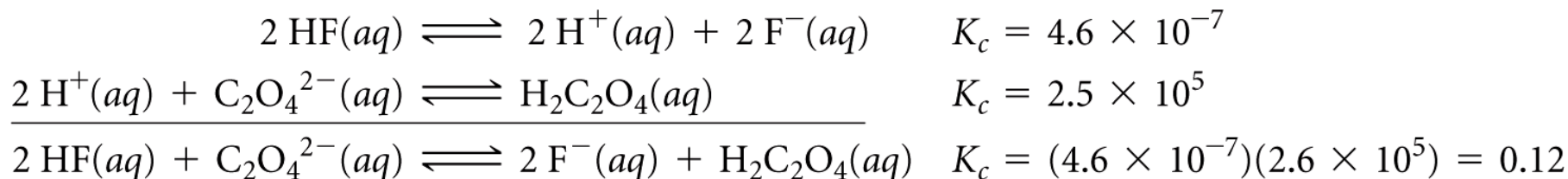
If we multiply the first equation by 2 and make the corresponding change to its equilibrium constant (**raising to the power 2**), we get



Reversing the second equation and again making the corresponding change to its equilibrium constant (**taking the reciprocal**) gives



Now we have two equations that sum to give the net equation, and we can multiply the individual K_c values to get the desired equilibrium constant.



➤ The Concentrations of Solids and pure Liquids Are Essentially Constant

- ❑ Because equilibrium-constant expressions includes terms only for reactants and products whose concentrations can change during a chemical reaction.
- ❑ Both the concentrations of solids and pure liquids (H_2O) can be obtained by multiplying the density of the substance by its molar mass—and both of these are constants at constant temperature.

➤ The Concentrations of Solids and Liquids Are Essentially Constant

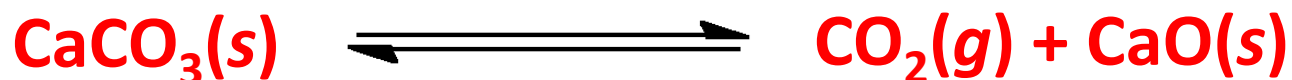
- Therefore, the concentrations of solids and liquids do not appear in the equilibrium expression.



$$K_c = [\text{Pb}^{2+}] [\text{Cl}^{-}]^2$$

➤ The Concentrations of Solids and Liquids Are Essentially Constant

- As long as *some* CaCO_3 or CaO remain in the system, gas pressures are the same, thus the amount of CO_2 above the solid will remain the same.

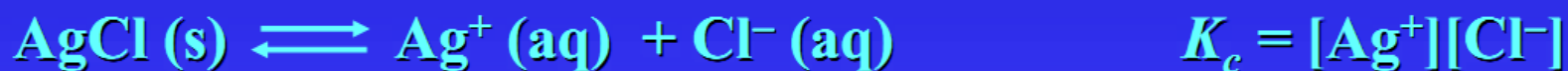
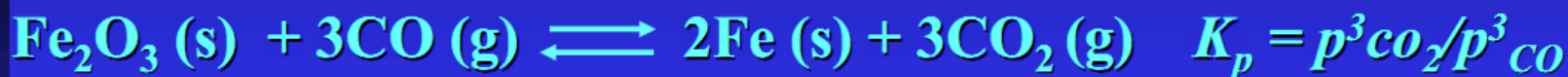
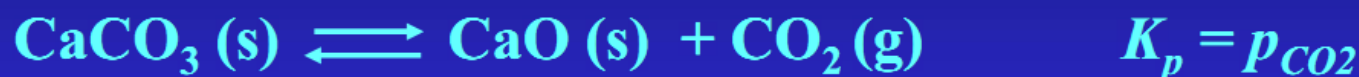


Large amount of CaCO_3 ,
small amount of CaO ,
gas pressure P



Small amount of CaCO_3 ,
large amount of CaO ,
gas pressure still P

5) 当有气体（或溶液）与固体共存于一个体系之中时，此类反应叫多相反应，它们的平衡叫多相平衡。此时，固相不必写入平衡常数式。（固相的平衡蒸气压一定；纯物质固体和液体的活度为1）。



- 6) 由起始状态到平衡状态过程中，凡浓度或压力几乎保持恒定不变的物质项可不必写入平衡常数式，即把该项浓度(或压力)归并入常数项。

例如有水参加的电离反应，水的浓度变化不大，不必写入表达式：



$$K = \frac{[\text{H}_3\text{O}^+][\text{Ac}^-]}{[\text{HAc}]}$$

Exercise Analyzing a Heterogeneous Equilibrium

Each of these mixtures was placed in a closed container and allowed to stand:

- (a) $\text{CaCO}_3(\text{s})$
- (b) $\text{CaO}(\text{s})$ and $\text{CO}_2(\text{g})$ at a pressure greater than the value of K_p
- (c) $\text{CaCO}_3(\text{s})$ and $\text{CO}_2(\text{g})$ at a pressure greater than the value of K_p
- (d) $\text{CaCO}_3(\text{s})$ and $\text{CaO}(\text{s})$

Determine whether or not each mixture can attain the equilibrium.

Solution

Plan For equilibrium to be achieved, it must be possible for both the forward process and the reverse process to occur.

Solve Equilibrium can be reached in all cases except (c) as long as sufficient quantities of solids are present.

(a) CaCO_3 simply decomposes, forming $\text{CaO}(\text{s})$ and $\text{CO}_2(\text{g})$ until the equilibrium pressure of CO_2 is attained. There must be enough CaCO_3 , however, to allow the CO_2 pressure to reach equilibrium. (b) CO_2 continues to combine with CaO until the partial pressure of the CO_2 decreases to the equilibrium value. (c) There is no CaO present, so equilibrium cannot be attained because there is no way the CO_2 pressure can decrease to its equilibrium value (which would require some of the CO_2 to react with CaO). (d) The situation is essentially the same as in (a): CaCO_3 decomposes until equilibrium is attained. The presence of CaO initially makes no difference.

Write the equilibrium-constant expression for the evaporation of water, $\text{H}_2\text{O}(l) \rightleftharpoons \text{H}_2\text{O}(g)$, in terms of partial pressures.

A. $K_p = 1/[\text{H}_2\text{O}(g)]$

☒ B. $K_p = P_{\text{H}_2\text{O}(g)}$

C. $K_p = [\text{H}_2\text{O}(g)]$

D. $K_p = 1/P_{\text{H}_2\text{O}(g)}$

Write the equilibrium-constant expression for the reaction $\text{NH}_3(aq) + \text{H}_2\text{O}(l) \rightleftharpoons \text{NH}_4^+(aq) + \text{OH}^-(aq)$

A. $K_c = [\text{NH}_4^+][\text{OH}^-]$

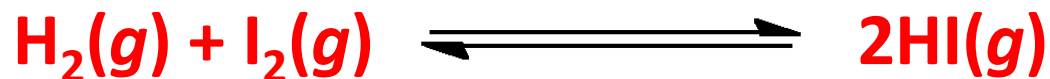
B. $K_c = \frac{[\text{NH}_4^+][\text{OH}^-]}{[\text{NH}_3]}$

C. $K_c = \frac{[\text{NH}_4^+][\text{OH}^-]}{[\text{NH}_3][\text{H}_2\text{O}]}$

D. $K_c = \frac{[\text{NH}_3][\text{H}_2\text{O}]}{[\text{NH}_4^+][\text{OH}^-]}$

➤ An Equilibrium Problem

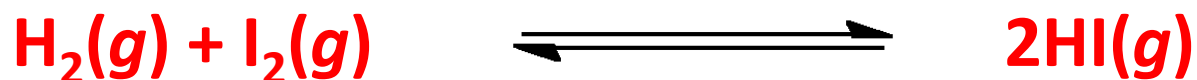
- A closed system initially containing $1.000 \times 10^{-3} \text{ M H}_2$ and $2.000 \times 10^{-3} \text{ M I}_2$ at 448°C is allowed to reach equilibrium. Analysis of the equilibrium mixture shows that the concentration of HI is $1.87 \times 10^{-3} \text{ M}$. Calculate K_c at 448°C for the reaction taking place, which is



➤ What Do We Know?

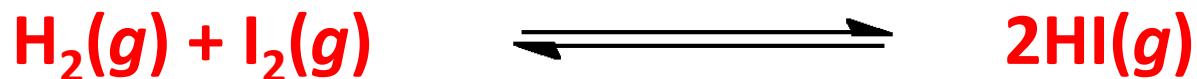
- ICE chart, where **ICE** stands for **I**nitial – **C**hange – **E**quilibrium

	$[\text{H}_2], M$	$[\text{I}_2], M$	$[\text{HI}], M$
Initially	1.000×10^{-3}	2.000×10^{-3}	0
Change			
At equilibrium			1.87×10^{-3}



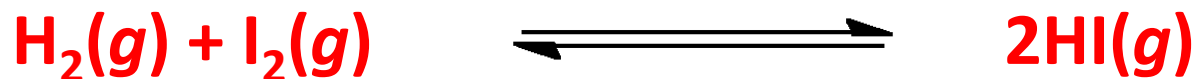
□ [HI] Increases by $1.87 \times 10^{-3} \text{ M}$

	$[\text{H}_2], \text{M}$	$[\text{I}_2], \text{M}$	$[\text{HI}], \text{M}$
Initially	1.000×10^{-3}	2.000×10^{-3}	0
Change			$+1.87 \times 10^{-3}$
At equilibrium			1.87×10^{-3}



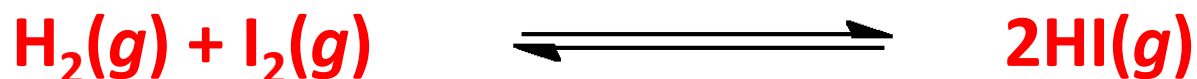
- Stoichiometry tells us $[H_2]$ and $[I_2]$ decrease by half as much.

	$[H_2], M$	$[I_2], M$	$[HI], M$
Initially	1.000×10^{-3}	2.000×10^{-3}	0
Change	-9.35×10^{-4}	-9.35×10^{-4}	$+1.87 \times 10^{-3}$
At equilibrium			1.87×10^{-3}



- We can now calculate the equilibrium concentrations of all three compounds

	$[\text{H}_2], M$	$[\text{I}_2], M$	$[\text{HI}], M$
Initially	1.000×10^{-3}	2.000×10^{-3}	0
Change	-9.35×10^{-4}	-9.35×10^{-4}	$+1.87 \times 10^{-3}$
At equilibrium	6.5×10^{-5}	1.065×10^{-3}	1.87×10^{-3}



□ and, therefore, the equilibrium constant:

$$\begin{aligned}K_c &= \frac{[\text{HI}]^2}{[\text{H}_2] [\text{I}_2]} \\&= \frac{(1.87 \times 10^{-3})^2}{(6.5 \times 10^{-5})(1.065 \times 10^{-3})} \\&= 51\end{aligned}$$

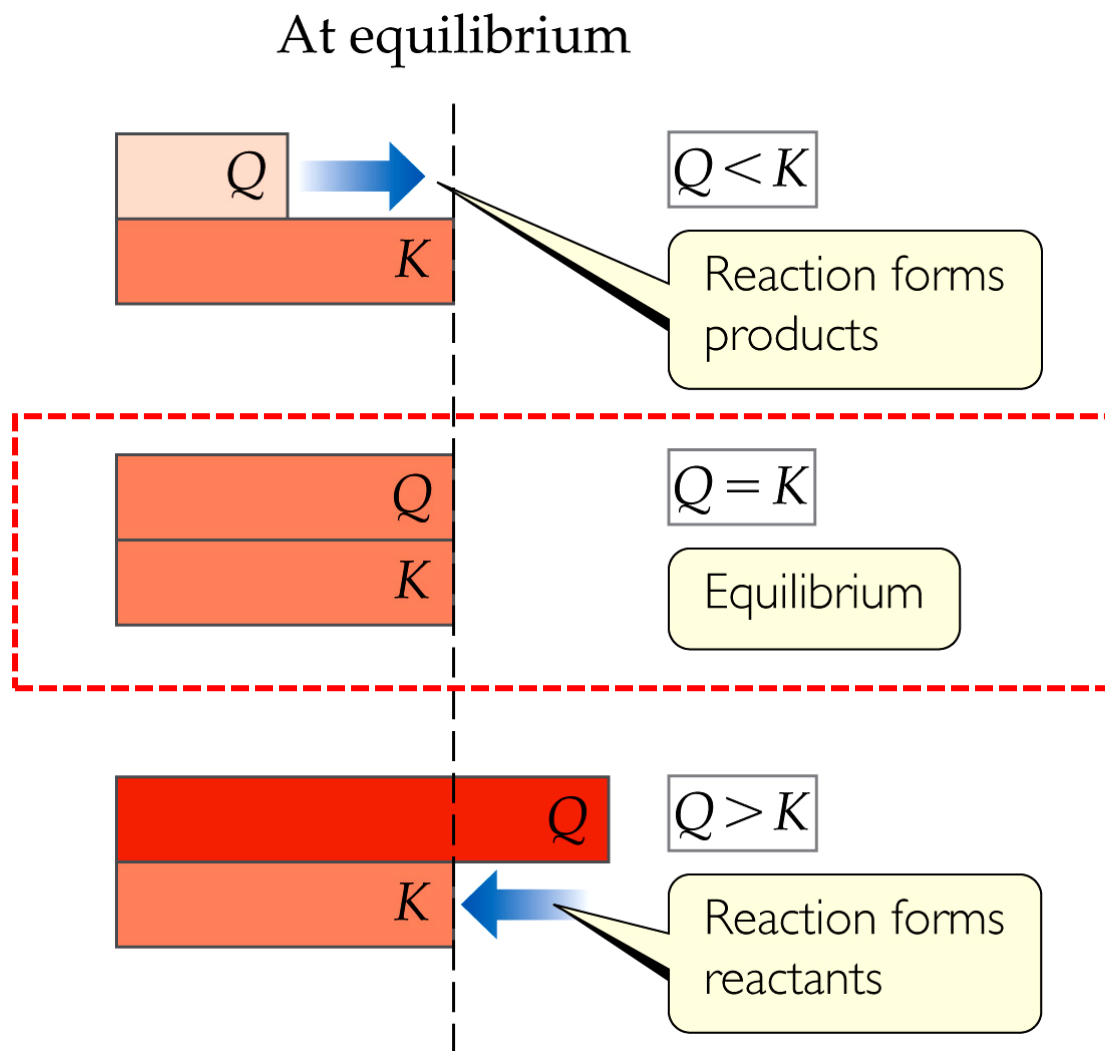
➤ The Reaction Quotient (反应商 Q)

- Q gives the same ratio the equilibrium expression gives, but for a system that is *not* at equilibrium.

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

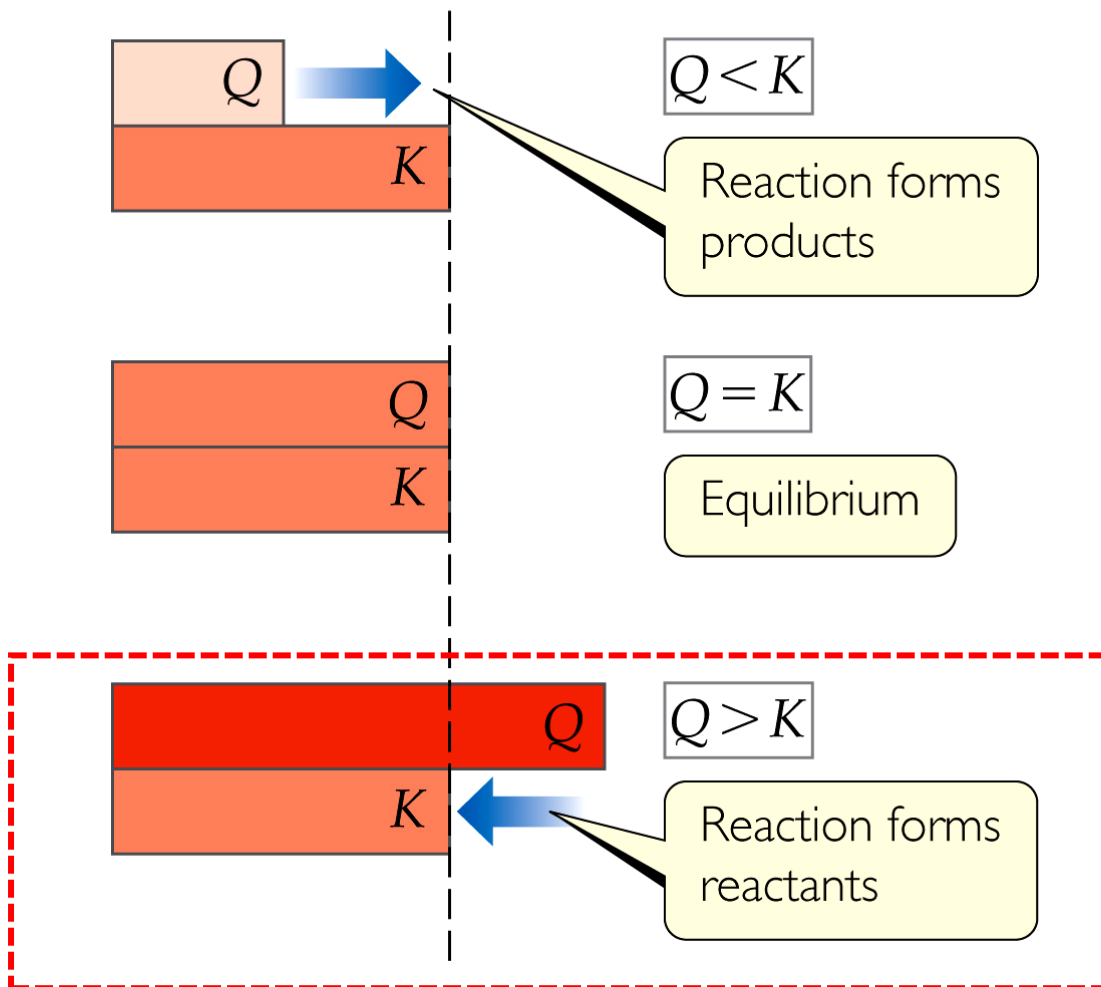
- To calculate Q , one substitutes the initial concentrations on reactants and products into the equilibrium expression.

□ If $Q = K$, the system is at equilibrium.



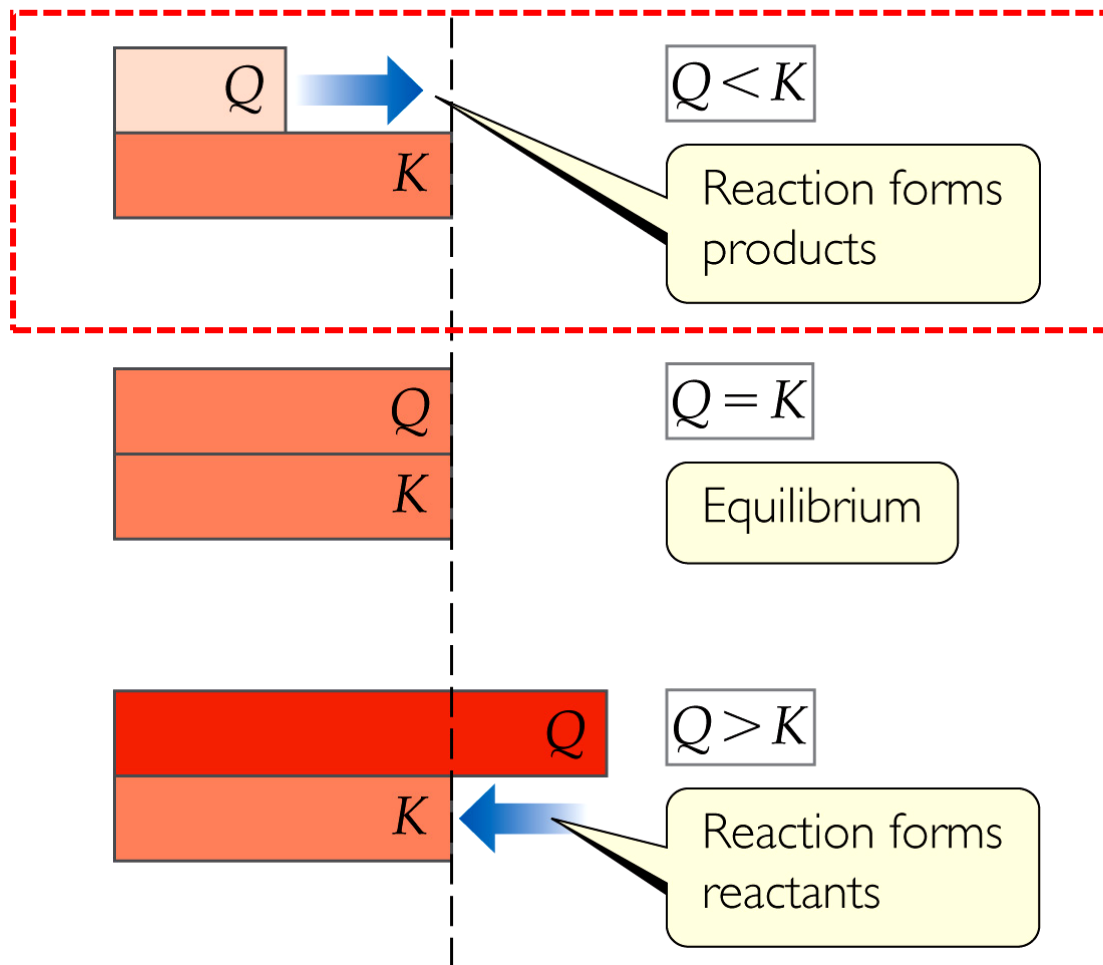
- If $Q > K$, there is too much product, and the equilibrium shifts to the left.

At equilibrium



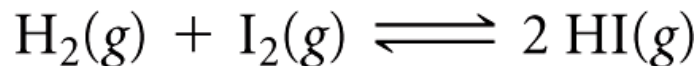
- If $Q < K$, there is too much reactant, and the equilibrium shifts to the right.

At equilibrium



Exercise Predicting the Direction of Approach to Equilibrium

At 448 °C the equilibrium constant K_c for the reaction



is 50.5. Predict in which direction the reaction proceeds to reach equilibrium if we start with 2.0×10^{-2} mol of HI, 1.0×10^{-2} mol of H_2 , and 3.0×10^{-2} of I_2 in a 2.00-L container.

Solution

The initial concentrations are

$$\begin{aligned} [\text{HI}] &= 2.0 \times 10^{-2} \text{ mol}/2.00 \text{ L} = 1.0 \times 10^{-2} \text{ M} \\ [\text{H}_2] &= 1.0 \times 10^{-2} \text{ mol}/2.00 \text{ L} = 5.0 \times 10^{-3} \text{ M} \\ [\text{I}_2] &= 3.0 \times 10^{-2} \text{ mol}/2.00 \text{ L} = 1.5 \times 10^{-2} \text{ M} \end{aligned}$$

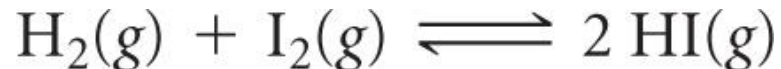
The reaction quotient is therefore

$$Q_c = \frac{[\text{HI}]^2}{[\text{H}_2][\text{I}_2]} = \frac{(1.0 \times 10^{-2})^2}{(5.0 \times 10^{-3})(1.5 \times 10^{-2})} = 1.3$$

Because $Q_c < K_c$, the concentration of HI must increase and the concentrations of H_2 and I_2 must decrease to reach equilibrium; the reaction as written proceeds left to right to attain equilibrium.

Exercise Calculating Equilibrium Concentration from Initial Concentrations

A 1.000-L flask is filled with 1.000 mol of $\text{H}_2(\text{g})$ and 2.000 mol of $\text{I}_2(\text{g})$ at 447 °C. The value of the equilibrium constant K_c for the reaction



at 447 °C is 50.5. What are the equilibrium concentrations of H_2 , I_2 , and HI in moles per liter?

Solution

First, we note the initial concentrations of H_2 and I_2 :

$$[\text{H}_2] = 1.000 \text{ M and } [\text{I}_2] = 2.000 \text{ M}$$

Second, we construct a table in which we tabulate the initial concentrations:

	$\text{H}_2(\text{g})$	+	$\text{I}_2(\text{g})$	\rightleftharpoons	$2 \text{HI}(\text{g})$
Initial concentration (M)	1.000		2.000		0
Change in concentration (M)					
Equilibrium concentration (M)					

Exercise Calculating Equilibrium Concentration from Initial Concentrations

Third, we use the stoichiometry of the reaction to determine the changes in concentration that occur as the reaction proceeds to equilibrium. The H_2 and I_2 concentrations will decrease as equilibrium is established and that of HI will increase. Let's represent the change in concentration of H_2 by x . The balanced chemical equation tells us the relationship between the changes in the concentrations of the three gases. For each x mol of H_2 that reacts, x mol of I_2 are consumed and $2x$ mol of HI are produced:

	$\text{H}_2(\text{g})$	+	$\text{I}_2(\text{g})$	\rightleftharpoons	$2 \text{HI}(\text{g})$
Initial concentration (M)	1.000		2.000		0
Change in concentration (M)	$-x$		$-x$		$+2x$
Equilibrium concentration (M)					

Fourth, we use initial concentrations and changes in concentrations, as dictated by stoichiometry, to express the equilibrium concentrations. With all our entries, our table now looks like this:

	$\text{H}_2(\text{g})$	+	$\text{I}_2(\text{g})$	\rightleftharpoons	$2 \text{HI}(\text{g})$
Initial concentration (M)	1.000		2.000		0
Change in concentration (M)	$-x$		$-x$		$+2x$
Equilibrium concentration (M)	$1.000 - x$		$2.000 - x$		$2x$

Exercise Calculating Equilibrium Concentration from Initial Concentrations

Fifth, we substitute the equilibrium concentrations into the equilibrium-constant expression and solve for x :

$$K_c = \frac{[\text{HI}]^2}{[\text{H}_2][\text{I}_2]} = \frac{(2x)^2}{(1.000 - x)(2.000 - x)} = 50.5$$

If you have an equation-solving calculator, you can solve this equation directly for x . If not, expand this expression to obtain a quadratic equation in x :

$$4x^2 = 50.5(x^2 - 3.000x + 2.000)$$

$$46.5x^2 - 151.5x + 101.0 = 0$$

Solving the quadratic equation (Appendix A.3) leads to two solutions for x :

$$x = \frac{-(-151.5) \pm \sqrt{(-151.5)^2 - 4(46.5)(101.0)}}{2(46.5)} = 2.323 \text{ or } 0.935$$

When we substitute $x = 2.323$ into the expressions for the equilibrium concentrations, we find *negative* concentrations of H_2 and I_2 . Because a negative concentration is not chemically meaningful, we reject this solution. We then use $x = 0.935$ to find the equilibrium concentrations:

$$[\text{H}_2] = 1.000 - x = 0.065 \text{ M}$$

$$[\text{I}_2] = 2.000 - x = 1.065 \text{ M}$$

$$[\text{HI}] = 2x = 1.87 \text{ M}$$