Chem 1062

Note Title 7/17/2008

* Lab Project Information Now Posted
* Lab Partners & Lab Reports
* D2L Homework Quizzes – Ch. 12, 14, 15

From end of lecture yesterday:

Reactions usually occur in a series of steps. Each step is limited to one, two, or three molecules reacting (colliding) at once. Each step in this process is called an elemtary reaction. The series of steps is called the reaction mechanism.

* Example: The decomposition of H_2O_2

Uncatalyzed:

activated complex

1) $H_2O_2 \rightarrow H_2O_2^{\ddagger}$ (slow)

2) $H_2O_2^{\ddagger} \rightarrow H_2O + O$ (fast)

3) $H_2O_2 + O \rightarrow H_2O + O_2$ (fast)

overall: $2H_2O_2 \rightarrow 2H_2O + O_2$

intermediate – produce in an earlier, consumed in a later step

unimolecular, bimolecular, termolecular

rate-determining step - slowest step in in a multistep process

catalyzed:

1) $H_2O_2 + \cancel{I^-} \rightarrow H_2O + \cancel{OI^-}$

2) $H_2O_2 + \cancel{OI^-} \rightarrow H_2O + O_2 + \cancel{I^-}$

$$2H_2O_2 \xrightarrow{I^-} 2H_2O + O_2$$

intermediate ⇒ OI^-

catalyst ⇒ I^-

Catalyst - consumed in an early step & produced in a later step

A catalyst speeds up a reaction by lowering the activation energy.

Ch. 15 - Chemical Equilibrium

What is it that is equal at equilibrium?

$$aA + bB \rightleftharpoons cC + dD$$

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

In a reaction, 0.600 mol N_2 and 1.200 mol H_2 were combined. If there were 0.040 mol NH_3 present @ equilibrium, how many moles of the other substances would be present @ equilibrium?

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

moles	N_2	$3H_2$	$2NH_3$
Initial	0.600	1.200	0
Change	$-x$	$-3x$	$+2x$
Equil	$0.600-x$ = 0.580	$1.200-3x$ = 1.140	$2x$ = 0.040

(1)

$$\frac{2x}{2} = \frac{0.040}{2}$$

$$x = 0.020$$

$0.600 - x = 0.600 - 0.020 =$

$1.200 - 3x = 1.200 - 3(0.020) = 1.140$

@ Equil: 0.580 mol N_2, 1.140 mol H_2, 0.040 mol NH_3

$$aA + bB \rightleftharpoons cC + dD$$

a, b, c, d ✓ represent coefficients

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

K_c ← equilibrium constant

Law of Mass Action

Important!

Kinetics: x, y, z – determined experimentally

$$aA + bB \xrightarrow{C} dD + eE$$

$$\text{Rate} = k[A]^x[B]^y[C]^z$$

Write an equilibrium constant expression for:

$$N_2(g) + 3H_2(g) \rightleftharpoons 2NH_3(g)$$

Then calculate the equilibrium constant for problem (1), assuming the reaction took place in a container having a volume of 15.0 L.

@ Equil: $\frac{0.580 \text{ mol } N_2}{15.0 \text{ L}}$, $\frac{1.140 \text{ mol } H_2}{15.0 \text{ L}}$, $\frac{0.040 \text{ mol } NH_3}{15.0 \text{ L}}$

0.03867 M N_2 ; 0.0760 M H_2 ; 0.002667 M NH_3

$$K_c = \frac{[NH_3]^2}{[N_2][H_2]^3} = \frac{(0.002667 M)^2}{(0.03867 M)(0.0760 M)^3}$$

$$K_c = 0.419$$

Heterogenous Equilibria

$$C(s) + 2N_2O(g) \rightleftharpoons CO_2(g) + 2N_2(g)$$

Write K_c expression:

$$K_c = \frac{[CO_2][N_2]^2}{[N_2O]^2}$$

leave out (l), (s) !!

(15.4) $HCN(aq) \rightleftharpoons H^+(aq) + CN^-(aq)$ $\quad$ $K_c = ?$

(1) $HCN(aq) + \cancel{OH^-(aq)} \rightleftharpoons CN^-(aq) + \cancel{H_2O(l)}$ $\quad K_1 = 4.9\times10^4$

(2) $\cancel{H_2O(l)} \rightleftharpoons H^+(aq) + \cancel{OH^-(aq)}$ $\quad K_2 = 1.0\times10^{-14}$

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(3) $HCN(aq) \rightleftharpoons H^+(aq) + CN^-(aq)$ $\quad K_3 = K_1 \cdot K_2$

$K_3 = 4.9\times10^{-10}$

$$K_1 \times K_2 = K_3$$

$$\frac{[CN^-]}{[HCN]\cancel{[OH^-]}} \times [H^+]\cancel{[OH^-]} = \frac{[H^+][CN^-]}{[HCN]}$$

(4)

$H^+(aq) + CN^-(aq) \rightleftharpoons HCN(aq)$ $\quad K_4 = \frac{1}{K_3}$

$$K_4 = \frac{[HCN]}{[H^+][CN^-]}$$

$K_4 = \frac{1}{4.9\times10^{-10}}$

$K_4 = 2.0\times10^9$

Qualitative Interpretation of Equilibrium Constant

K_c is small, reactant-favored

K_c is large, product-favored

Predicting the Direction of a Reaction for a system that is not at equilibrium:

$$aA + bB \rightleftharpoons cC + dD$$

Find the Q_c (reaction quotient)

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

(15.56) $CH_4(g) + 2H_2S(g) \rightleftharpoons CS_2(g) + 4H_2(g)$

$K_c = 3.59$ @ 900°C

a) $[CH_4] = 1.26\,M$ $\quad [H_2S] = 1.32\,M$

$[CS_2] = 1.43\,M$ $\quad [H_2] = 1.12\,M$

$$Q_c = \frac{[CS_2][H_2]^4}{[CH_4][H_2S]^2} = \frac{(1.43)(1.12)^4}{(1.26)(1.32)^2}$$

$$= 1.02$$

not at equilibrium, goes to the right

If $Q_c = K_c$, then at equilibrium.

$Q_c < K_c$, then reaction goes to right

$Q_c > K_c$, " " " " left

(15.60) $N_2(g) + O_2(g) \rightleftharpoons 2NO(g)$

$K_c = 0.0025$ @ 2127°C

$[N_2] = 0.023\,M$; $[O_2] = 0.031\,M$

$[NO] = ?$

$$[N_2][O_2]K_c = \sqrt{\frac{[NO]^2}{[N_2][O_2]}} = (0.023)(0.031)(0.0025)$$

$$= \sqrt{1.7825 \times 10^{-6}}$$

$[NO] = 0.0013\ M$

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(62) do this one for Monday