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First Class

General Chemistry

Chemical reaction

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Chemical reaction

<u>Chemical reaction</u>: In a chemical change, the reading substances change into new substances that have different formulas and different properties. A chemical reaction always involves chemical change becomes atoms of the reacting substances, form new combination with new properties. A chemical equation uses symbols & formulas to represent a chemical reaction. The substances on the left side of the equation are called reactants, & those on the right side are called products.

<u>Types of chemical reaction</u>: chemical reactions can be divided into 1.Combination reaction, 2. Decomposition reaction, 3. Single replacement or substitution reactions, 4. and Double displacement. These are illustrated in table 1.

Table 1. Chemical reactions		
Type	General equation	Example
Combination	$A + B \longrightarrow AB$	$C + O_2 \longrightarrow CO_2$
		$2S + 3O_2 \longrightarrow 2SO_3$
Decomposition	$AB \longrightarrow A + B$	$2HgO \longrightarrow 2Hg + O_2$
		$2\text{KClO}_3 \longrightarrow 2\text{KCl} + 3\text{O}_2$
Single replacement	$A + BC \longrightarrow AC + B$	$Zn + CuSO_4 \longrightarrow ZnSO_4 + Cu$
	or	
	$A + BC \longrightarrow BA + C$	$Cl_2 + 2NaBr \longrightarrow 2NaCl + Br_2$
Double displacement	$AB + CD \longrightarrow AD +$	$Na_2SO_4 + BaCl_2 \longrightarrow 2NaCl + BaSO_4$
	CB	
		$FeS + 2HCl \longrightarrow FeCl_2 + H_2S$

Table 1. Chemical reactions

Equilibrium reactions: Many times when two or more reactants are unite to form a certain number of products, these products themselves unite to reform the original reactants. Reaction of this type is called **reversible reactions**. They are indicated by a double arrows \iff showing that the reaction may proceed in either direction depending upon the conditions that exist.

If we start with a mixture of N_2 and H_2 . At a given *temperature* and *pressure* (with a *catalyst*) we will soon have some NH_3 formed. As more NH_3 is formed, it will begin to decompose into N_2 and H_2 .

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

When the rates of formation and decomposition become equal, **a chemical** *equilibrium* exists. An equilibrium may be-

defined as a dynamic state in which the rate of the forward reaction is equal to the rate of the reverse reaction.

Two examples of equilibrium reactions in the body are

$$HCO_3 + H^+ \rightleftharpoons H_2CO_3 \rightleftharpoons CO_2 + H_2O$$

and

hemoglobin + oxygen \iff oxyhemoglobin

equilibrium constant (law of mass action): Consider the following general equilibrium reaction.

 $aA + bB \longrightarrow cC + dD$

The <u>law of mass action</u> states that the rate of a chemical reaction is proportional to the concentration of the reacting substances. So, for the above reaction, rate forward equal to the = $k_1[A]^a[B]^b$ where k_1 is proportionality constant and the brackets, [], indicate concentrations in the units **moles/liter** .likewise, the rate of the reverse reaction = $k_2[C]^c[D]^d$ where k_2 another proportionality constant.

At equilibrium, the rate of the forward reaction is equal to the rate of the reverse reaction, so

$$K_1 \ge [A]^a \ge [B]^b = k_2 \ge [C]^c \ge [D]^d$$

Whence

$$\frac{\left[\mathrm{C}\right]^{\mathrm{c}} \mathrm{x} \left[\mathrm{D}\right]^{\mathrm{d}}}{\left[\mathrm{A}\right]^{\mathrm{a}} \mathrm{x} \left[\mathrm{B}\right]^{\mathrm{b}}} = \frac{k_{1}}{k_{2}} = k_{\mathrm{eq}}$$

In general, the equilibrium constant, K_{eq} , equals the product of the products concentration divided by the product of the reactants concentration, each

concentration raised to the power indicated by *its coefficient* in the equation. So. For the reaction as follows:

 $4A + 3C \implies 2D + F$

$$K_{eq} = \frac{[D]^2[F]}{[A]^4[C]^3}$$

Ex1: In the conversion of glucose to vitamin C, the following reaction take place.

 $\begin{array}{ccc} C_5H_{11}O_5COOH & \longleftarrow & H^+ & + & C_5H_{11}O_5COO \\ \hline gluconic acid & hydrogen ion & gluconate ion \\ \end{array}$

In the equilibrium concentrations in moles per liter are C₅H₁₁O₅COOH, 0.10; H⁺, 3.7 x 10⁻³; C₅H₁₁O₅COO, 3.7 x 10⁻³, calculate the value of K_{eq} .

 $K_{eq} = [H^+] \times [C_5 H_{11} O_5 COO^-] / [C_5 H_{11} O_5 COOH]$

 $K_{\rm eq} = (3.7 \text{ x } 10^{-3}) \text{ x } (3.7 \text{ x } 10^{-3}) / 0.10 = 1.4 \text{ x } 10^{-4}$

Ex2:In manufacturing of wood alcohol, the following equilibrium reaction occurs;

CO + 2H₂ \Rightarrow CH₃OH. At equilibrium the concentrations in moles per liter are CO, 0.025 ; H₂ 0.050; CH₃OH, 0.12; calculate the value of K_{eq} .

 $K_{eq} = [CH_3OH] / [CO] \times [H_2]^2 = (0.12) / (0.025) \times (0.050)^2 = 1.9 \times 10^3$

In general, a large value of K_{eq} indicates an equilibrium that has been shifted far to the right, whereas a small value indicates one shifted to the left.

Le Chatelier's Principle: Le Chatelier's principle states that *if a stress is applied to a reaction at equilibrium, the equilibrium will be displaced in such a direction as to relieve the stress.* Stresses are 1. Effect of concentration 2. Effect of temperature 3. Effect of a catalyst.

<u>A catalyst</u>: Any substance that increase the speed of a reaction without itself being changed chemically is called <u>catalyst</u>. Those catalysts present in the body called <u>enzymes</u>. During digestion, for example, the foods undergo many chemical

changes, each under the influence of a specific enzyme. There are also <u>inhibitors</u> that slow down rather than speed up chemical reactions.

Reaction Rates: Some chemical reactions proceed at a slow rate. Iron, for example, rusts very slowly. Wood takes years to decay. On the other hand, some chemical reactions proceed more rapidly. Coal burns steadily and quickly. Concrete begins to set within a few hours. Some chemical reactions not only occur rapidly, they take place almost instantaneously. Consider the violent explosion of dynamite. Within a fraction of a second, the complete reaction has take place.

What determines the speed of a chemical reaction? The speed of a chemical reaction depends upon several factors: (1) the nature of the reacting substances, (2) the temp.,

(3) the concentration of the reacting substances, (4) the presence of a catalyst, and (5) the surface area.

Temperature: A patient who has a fever of only a few degrees has an increased pulse rate and also an increased respiratory rate. Reactions taking place throughout the body proceed at an accelerated rate.

When the temperature of the human body drops, the various metabolic processes slow down. This fact is of great importance, for example, during openheart surgery.

The rate of chemical reaction :

$$aA + bB \leftrightarrow cC + dD$$

$$Rate = \frac{-d[A]}{dt} \quad or \quad \frac{-d[B]}{dt}$$

$$Rate = \frac{+d[C]}{dt} \quad or \quad \frac{+d[D]}{dt}$$

$$or \; Rate \; of \; reactant = \frac{-\Delta c}{\Delta t}$$

$$or \; Rate \; of \; product = \frac{+\Delta c}{\Delta t}$$

The Arrhenius Equation

• Arrhenius discovered most reaction-rate data obeyed the equation:

 $k = Ae^{-Ea/RT}$

• **k** is the rate constant, **E**_a is the activation energy, **R** is the gas constant (8.314 J/K-mol) and **T** is the temperature in K

A is called the frequency factor. A is a measure of the probability of a favorable collision.

Both A and E_a are specific to a given reaction.

• E_a can be determined and graphically :

$$\begin{array}{rcl}
\ln k & = & -\underline{E}_{\underline{a}} + \ln A \\
& & RT
\end{array}$$

• Or Ea can be determined if the rates of chemical reactions are known for two given temperatures:

$$\ln \frac{\mathbf{k}_1}{\mathbf{k}_2} = \begin{vmatrix} \underline{\mathbf{E}}_a & \underline{\mathbf{1}} \\ \mathbf{R} & \mathbf{T}_2 \end{vmatrix} - \begin{vmatrix} \underline{\mathbf{1}} \\ \mathbf{T}_1 \end{vmatrix}$$

Activation energy, E_a , is the minimum energy required to initiate a chemical reaction .

• In order to form products, bonds must be broken in the reactants. Bond breakage requires energy



