Environmental Engineering

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Chapter 1 Introduction to environmental engineering and problem solving

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Chapter 1 Introduction to environmental engineering and problem solving

● HOMEWORK

Example （Page21-23）

Chapter 1 Introduction to environmental engineering and problem solving

- 1.5.2 Using tables and figures to analyze and communicate results

Tables and figures can be used as powerful tools to analyze and to communicate the physical context of your results. When using these visual communication tools, the honest documentation of your results is crucial. Avoid the dangers associated with forcing your data to fit your anticipated results. Report them as simply and honestly as possible.

Although reported data within a figure or a table provides an excellent visual summary, it does not substitute for the complete discussion of your results; showing results in a table or a figure only is inadequate. Discussion of your findings as presented in the figure is still necessary.

Chapter 1 Introduction to environmental engineering and problem solving

1.5.2 Using tables and figures to analyze and communicate results

Table 1.6 provides an example of the type of data that are easily communicated in tabular form. The table provides a list of polycyclic aromatic hydrocarbons (PAHs) (多环芳烃) **having environmental interest in relation to their molecular weight, solubility, and soil-water partition coefficient.** Polycyclic aromatic hydrocarbons are comprised of fused benzene rings（稠合苯环）, are found in gasoline, are prevalent in the environment as a result of incomplete combustion of fossil fuels, and are characteristic of the hydrocarbons found in coal tar（煤焦油）. **Important factors that may influence the environmental fate of a PAH compound include the compound's aqueous solubility(水溶性), its vapor pressure, and its soil-water partition coefficient.** In general, as the compound molecular weight increases, the more likely it is to absorb or adsorb to the solid phase, thus characterized by an increasing partition coefficient.

Table 1.6 Characteristics of polycyclic aromatic hydrocarbons with environmental significance.

Hydrocarbon	Molecular weight (g/mol)	Solubility (mg/L)	Soil-water partition coefficient
Benzene	78.11	1780	97
Toluene	92.1	500	242
o-xylene	106.17	170	363
Ethyl benzene	106.17	150	622
Naphthalene	128.16	31.7	1300
Acenophthene	154.21	3.93	2580
Acenaphthylene	152.2	3.93	3814
Fluorene	166.2	1.98	5835
Fluoranthene	202	0.275	19000
Phenanthrene	178.23	1.29	23000
Anthracene	178.23	0.073	26000
Pyrene	202.26	0.135	63000
Benzo(a)anthracene	228	0.014	125719
Benzo(a)pyrene	252.3	0.0038	282185
Chrysene	228.2	0.006	420108
Benzo(b)fluoranthe	252	0.0012	1148497
Benzo(g,h,i)perylene	276	0.00026	1488389
Dibenz(a,h)anthracene	278.35	0.00249	1668800
Benzo(k)fluoranthene	252	0.00055	2020971

Chapter 1 Introduction to environmental engineering and problem solving

1.5.2 Using tables and figures to analyze and communicate results

Engineers often use x-y graphs or scatterplots to communicate the strength of relationship between two variables. Pie and bar charts may also be useful given the nature of the data. When making a chart, maximize the effectiveness by incorporating as much related data as possible on a given figure without compromising clarity. For example, data in Figure 1.9 describe how acid yellow 17 dye concentration changes with respect to treatment time with ozone. Results are presented from three different experiments on this one figure to allow for comparison. Displaying data in this matter also allows for a visual representation of the relationship between variables. A review of Figure 1.9 provides some guidelines for effectively plotting experimental results. Note that the figure is clearly labeled at the bottom of the caption. The plot is descriptive, yet simple, and the x-and y-axes are clearly labeled and have associated numerical values with units.
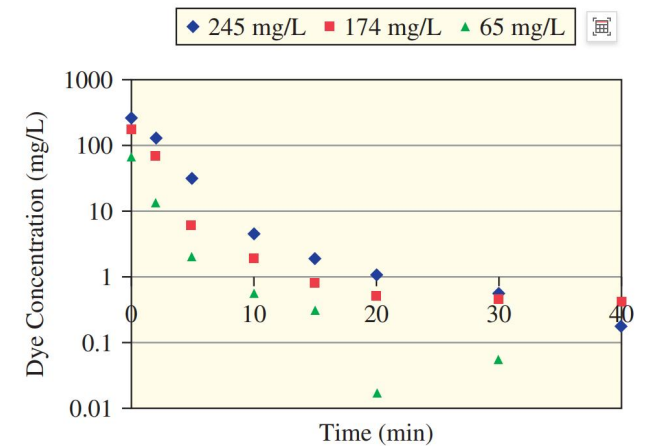

Figure 1.9 Example figure illustration that shows how dye concentration is changing as ozonation time increases.

Chapter 1 Introduction to environmental engineering and problem solving

1.5.3 Linear regression and the correlation coefficient（线性回归和相关系数）

Scatterplots (x-y graphs) are useful **to view the form, direction, and strength of relationship between two variables.** Often, the relationship is linear. The correlation coefficient can be used to quantify both the direction and strength of the observed linear relationship, and it serves as a "goodness of fit" measure.

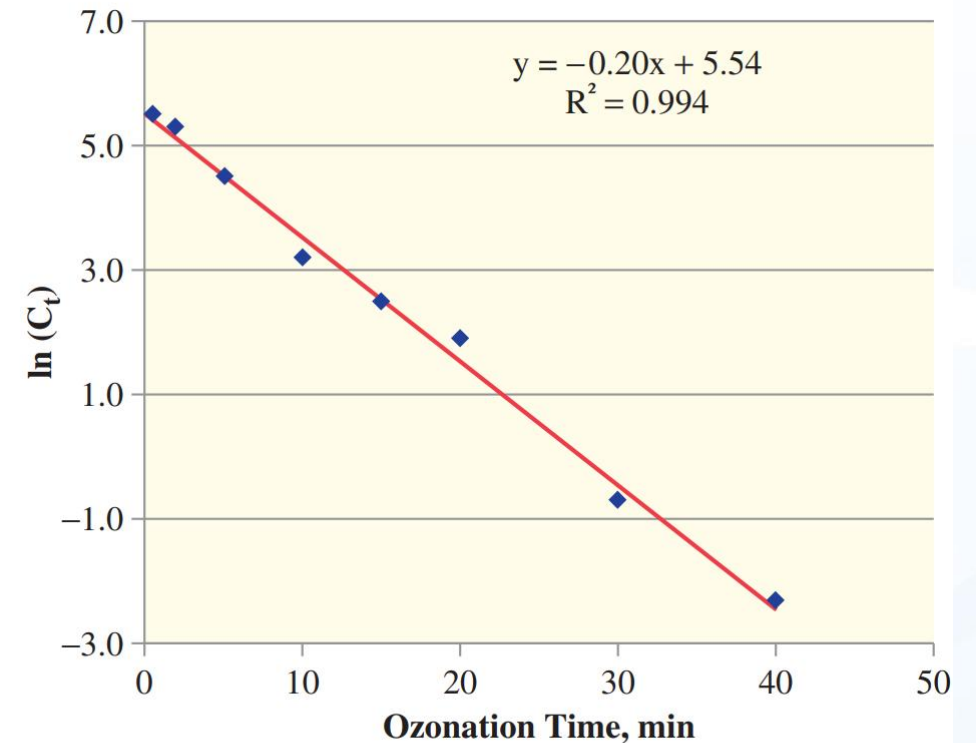The least-squares method（最小二乘法） is commonly used for fitting a regression line.

$$y = -0.20x + 5.54$$
$$R^2 = 0.994$$

Figure 1.14 Manipulate the first-order rate equation and use experimental results to determine the rate coefficient, k.

1.5.4 Interpreting linear, power, and exponential equations （线性、幂和指数方程）

Many simple nonlinear functions can be algebraically manipulated into linear form.

There are many additional systems encountered by environmental engineers that are described using nonlinear models that can be easily manipulated into a linear format. For example, the Monod model (Monod, 1949), used to predict the state of a continuous flow bioreactor or chemostat, is described using two variables: the specific growth rate of the microbes (μ) and the growth-limiting substrate (S).

1.5.5 Student's t-test（学生t检验）

The Student t-test was invented by William Sealy Gosset and published under the pen name "Student" in 1908. There are one-sided t-test and two-sided t-test(单侧t检验和双侧t检验).

Student's t-test, sometimes are also called one-tailed t-test and two-tailed t-test , is used to compare the means of two sample groups by determining if the two groups are statistically different from each other. The t-test assumes that the measurements within the two groups are normally distributed and that the variances in the two groups are equal.

1.5.6 One-way analysis of variance (ANOVA)

The One-way Analysis of Variance (ANOVA) is a commonly used statistical method employed to detect differences of three or more means of grouped data. Like the Student t-test, the ANOVA method is used to test the equality of the means rather than to predict new values of a dependent variable (regression analysis is often used for this type of analysis).

Chapter 2 Essential chemistry concepts

Learning Objectives

After reading this chapter, you should be able to:

• understand the commonly used systems of units and the difference between fundamental and derived units;

• balance chemical equations and apply stoichiometry(化学计量学) to environmental applications.

• define what is meant by oxidation and reduction, and develop half-reactions for oxidation-reduction reactions;

• learn the fundamental concepts of thermodynamics and apply them to chemical equilibria (化学平衡).

• evaluate acid-base systems for determining pH and all chemical species involved at equilibrium; comprehend the importance of the carbonate system and be able to calculate the alkalinity of a water sample;

• calculate the solubility product(溶解度积（Ksp）) and determine if a solution is undersaturated(不饱和的), saturated, or supersaturated with respect to specific chemical species;

• explain the difference between the three major groups of hydrocarbons and explain the major functional groups of organic compounds and their importance in environmental engineering.

Chapter 2 Essential chemistry concepts

2.1 Introduction

- Environmental engineers and scientists must have a strong understanding of chemical concepts.

- Chemicals such as alum, lime, soda ash, and sodium hydroxide（氢氧化钠）are routinely added to hard water in order to precipitate calcium and magnesium ions.

- Ferrous sulfate（硫酸亚铁），ferric chloride（氯化铁），and lime may be added to wastewater for removing orthophosphate（正磷酸盐）.

- Chlorine and ozone are often used for oxidizing organic compounds and as primary disinfectants in various environmental applications.

- The gas laws are important, since oxygen or nitrogen may be added to a reactor to enhance biological oxidation or to strip out unwanted gases. The chemistry and solubility of gases such as carbon dioxide, oxygen, and ammonia in water affect the rate at which they can be transferred into or out of solution and the saturation concentration of each. The formation of smog and other photochemical species relates to atmospheric chemistry.

- As engineers, we are not only concerned about the final or equilibrium concentrations that can be achieved during a chemical reaction but, more importantly, the rate of reaction.

Chapter 2 Essential chemistry concepts

2.2 Dimensions, units, and conversions

● Specifically, physical quantities such as length, time, temperature, pressure, velocity, and weight are some of the most widely used measurements. These types of measurements are used to describe an object or system. Not only is it important to specify the magnitude or numerical value of the physical quantity, it is essential that the dimension being expressed be accompanied by the appropriate set of units. The units provide the increments necessary to quantify the dimension.

Chapter 2 Essential chemistry concepts

● 2.2 Dimensions, units, and conversions

● **2.2.1 Density**

● The density of a substance is defined as mass per unit volume.

● Example 2.1 The effect of impurities on the density of water (P45).

$$\rho = \frac{m}{\cancel{V}}$$

● **2.2.2 Specific gravity（比重）**

● Specific gravity is dimensionless.

● Example 2.2 Calculating speciffc gravity and density

$$\text{Specific Gravity (S.G.)} = \frac{\rho_{substance}}{\rho_{water\ at\ 4°C}}$$

Chapter 2 Essential chemistry concepts

2.2 Dimensions, units, and conversions

- **2.2.3 Concentrations**

- There are various ways to express the concentration of a substance in a solution: **mass or weight per unit volume,** mass or weight percentage, volume percent, moles per liter, mole fraction, and equivalents per liter. Each of these will be described briefly. Concentration is a derived dimension.

- Example 2.3 Calculating solution concentration (P47-48)

Chapter 2 Essential chemistry concepts

2.2 Dimensions, units, and conversions

● **2.2.4 Mass and volumetric flow rates（质量流量和体积流量）**

● In environmental engineering, the flow rate may be expressed either on a mass (gravimetric) or a volumetric basis. **The mass-based flow rate represents the quantity of mass flowing through a pipe or system per unit of time.** It is usually expressed in units such as kilograms per second (kg/s) or pounds per minute (lb/min).

● **Volumetric flow rate** refers to the volume of fluid passing through a section per unit of time. Common units include cubic meters per second (m^3/s), liters per minute (L/min), or gallons per minute (GPM). The measurement of volume flow is very important for applications such as liquid or gas transport, water treatment, etc.

● Example 2.4 Calculating mass flow rate (SI) units (P49)

● Example 2.5 Calculating mass flow rate (EE) units (P49)

Chapter 2 Essential chemistry concepts

2.2 Dimensions, units, and conversions

- 2.2.5 Detention time(滞留时间)

- A fundamental concept in environmental engineering is detention time. Traditionally, this is defined **as the average unit of time that a fluid particle remains in a system** (e.g., reactor, pipe, or tank). Alternatively, it is defined as the time required filling a tank or container. **Detention time is also known as retention time or residence time.** Mathematically, detention time is determined by dividing the volume of the tank or container by the volumetric flow rate (Q) as shown below.

$$\tau = \frac{V}{Q}$$

- Example 2.6 Calculating detention time (P50)

2.3 Balancing reactions

● A chemical equation expresses what happens during a chemical reaction or chemical change. **Instead of trying to explain in words what happens during a chemical reaction, chemical elements, compounds, and symbols are used to convey this in a clear and concise manner using a chemical equation.** Chemical equations must be verified by experimentation in the laboratory.

● Environmental engineers use chemical equations **for estimating the quantities of chemicals that are added to water, wastewater, sludge, contaminated gas streams, etc. For example, these equations can also be used to estimate the quantity of precipitate that is generated during softening of hard water.**

● Before using any chemical equation, **one must examine it closely to determine if the equation is properly balanced.** An equation is balanced when the law of conservation of mass is satisfied; i.e., the mass of all elements on both sides of the equation are the same and the net charge of all compounds is zero. It is important to remember that atoms are neither created nor destroyed during a chemical reaction.

● **A properly balanced equation represents the stoichiometry of the equation**; that is, it shows the relationship between the number moles of each reactant and the number of moles of the various products that are produced.

Chapter 2 Essential chemistry concepts

2.4 Oxidation-reduction reactions

●In oxidation-reduction or redox reactions, atoms or ions undergo a change in their oxidation number and this is always accompanied by a transfer in electrons. Recall that oxidation（氧化） is defined as the loss of electrons or a gain in valence(价电子). The opposite of oxidation is reduction（还原）, which is defined as a gain in electrons or a loss in valence, i.e., a loss in oxidation number.

$$Fe+Cu^{2+}\rightarrow Fe^{2+}+Cu$$
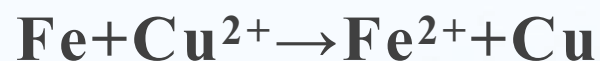
●If one element releases electrons, then another element must be present to accept the electrons.

●With these concepts in mind, an oxidizing agent is any substance that can add electrons. Alternatively, any substance that can give up electrons is called a reducing agent. Elements that have an intermediate oxidation state may serve either as an oxidizing or reducing agent.

2.4 Oxidation-reduction reactions

- Follow the steps presented below for balancing complex oxidation-reduction equations.

1 Check to see whether any chemical species is being oxidized or reduced.

2 Write and balance half-reactions.

3 Fill in the remainder of the chemical equation.

4 Check mass balance on both sides of the equation.

Table 2.9 Common oxidizing and reducing agents.

Oxidizing agents	Reducing agents
O(0)	H(0)
Cl(0)	Fe(0)
Fe(III)	Mg(0)
Cr(IV)	Fe(II)
Mn(IV)	Cr(II)
Mn(VII)	Mn(IV)
N(V)	N(III)
N(III)	Cl(−I)
S(0)	S(0)
S(IV)	S(−II)
S(VI)	S(IV)

Chapter 2 Essential chemistry concepts

2.5 Thermodynamic equilibrium

- Thermodynamics is the branch of science dealing with changes in energy that accompanies physical and chemical processes.

- Thermodynamics allows environmental engineers and chemists to determine whether or not a chemical reaction will or will not occur.

- However, it will not allow us to predict the rate of reaction.

- The thermodynamic laws allow us to predict equilibrium of a reaction.

- Other importance aspects of thermodynamics in environmental engineering relate to biological energetics, sludge drying and incineration, and the cooling of thermal wastes.

2.5 Thermodynamic equilibrium

2.5.1 First law of thermodynamics（热力学第一定律）

● The first law of thermodynamics states that energy may neither be created nor destroyed, only transferred or changed from one form to another. The change in internal energy of the system is related to the flow of heat into or out of the system and the work done by the system.

$$\Delta E = q - w$$

where: ΔE=change in internal energy of the system ;
q = heat added to the system;
w = work done by the system.

Chapter 2 Essential chemistry concepts

2.5 Thermodynamic equilibrium

2.5.1 First law of thermodynamics（热力学第一定律）

● When ΔE has a negative value, it means that the reaction is exothermic(放热 的) or heat is given off. A positive value for ΔE indicates an endothermic(吸 热的) reaction and that heat is absorbed. Most chemical reactions are not performed or conducted at a constant volume, but at a constant pressure of 1 atm. For constant pressure, it is necessary to define a new function of state, enthalpy (H，焓), as presented below.

$$H = E + PV$$

where: H = enthalpy of the system;
H = total energy content of an element or compound
E = internal energy of the system
P = pressure on the system
V = volume of the system.

Chapter 2 Essential chemistry concepts

2.5 Thermodynamic equilibrium

2.5.1 First law of thermodynamics（热力学第一定律）

● A change in enthalpy is expressed as:

$$\Delta H = \Delta E + \Delta(P \Psi)$$

$$\Delta H = q - w + \Delta(P \Psi)$$

● The total enthalpy of a system is difficult to measure, so scientists and engineers are generally interested in a change in enthalpy. A system has been developed so that the change in enthalpy, or the heat of formation of a compound or element, can be determined at standard conditions of 25◦ C and 1 atm pressure. At standard conditions, compounds whose standard state is gas, liquid, or crystal or solid are assigned enthalpies equal to zero.

Chapter 2 Essential chemistry concepts

2.5 Thermodynamic equilibrium

2.5.1 First law of thermodynamics（热力学第一定律）

●In chemical reactions, the first law helps us calculate the energy change of the reaction, including the heat of the reaction (exothermic or endothermic), the energy change during the phase transition, and so on. This is essential for designing chemical reactions, evaluating the feasibility of reactions, and predicting the effect of reaction conditions (e.g., temperature, pressure) on reactions.

Chapter 2 Essential chemistry concepts

2.5 Thermodynamic equilibrium

2.5.2 Second law of thermodynamics

The second law of thermodynamics states that all systems tend to approach a state of equilibrium. **Entropy（S,熵）** is the concept developed by physical chemists used to judge whether or not a chemical process is at equilibrium or proceeding to equilibrium. Work can only be obtained from systems that have not reached equilibrium. In a reversible process, the entropy of the universe is constant. In an irreversible process, the entropy of the universe increases. An increase in entropy relates to a decrease in the orderliness of a system, while a decrease in entropy causes an increase in the orderliness of the system.Changes in entropy at standard conditions (25° C) can be calculated using entropy values for the products and reactants in chemical reactions.

The second law guides our understanding of the direction and limits of chemical reactions. It tells us that even if a reaction is energetically possible (i.e. satisfies the first law), it will not necessarily occur spontaneously unless it leads to an increase in the total entropy of the system. The concept of entropy is also related to the spontaneity of the reaction, the equilibrium state of the reaction, and the rate of the reaction. **When designing a chemical reaction, the second law helps to predict whether the reaction will occur spontaneously and the concentration of the components when the reaction reaches equilibrium.**

2.5 Thermodynamic equilibrium

2.5.3 Gibbs free energy, ΔG

● **Free energy is that component of the total energy of a system which can do work under isothermal(等温条件) conditions. For irreversible processes(不可逆过程), ΔS increases; however, the change in free energy ΔG decreases.**

$$G = H - TS$$

where: G= Gibbs free energy
H =enthalpy of system
T = absolute temperature of system
S = entropy of system.

ΔG is an important criterion for determining the spontaneity of chemical reactions. Under isothermal and isobaric（等温等压） conditions, a process is spontaneous if the change in Gibbs free energy (ΔG) is less than zero (ΔG<0). If ΔG>0, the process is non-spontaneous and requires external energy input. When ΔG=0, the system reaches equilibrium.

Chapter 2 Essential chemistry concepts

2.5 Thermodynamic equilibrium

2.5.4 Extent of reaction, equilibrium constant (K)

● **The equilibrium constant (K) can be determined from free energy data.The equilibrium constant is dependent upon temperature.**

2.6 Acid-base chemistry

- Rather than expressing the hydrogen ion concentration in moles/L, Sorensen in 1909 proposed the concept of pH (Sawyer and McCarty, 1978). The pH scale is usually represented by a scale ranging from 0 to 14, with a neutral pH indicated by a value of 7. Solutions are acidic when the pH is below 7 and basic or alkaline when the pH is higher than 7. The pH of water at 25∘ C is equal to 7, therefore, it is neutral. Mathematically, pH is defined as the negative of the logarithm of the hydrogen ion concentration.

$$pH = -\log [H^+]$$

- The hydrogen ion concentration, as monitored by pH, is an important parameter in environmental engineering. Rates of biological and chemical reactions are impacted by pH and, outside a specific range, they may not proceed. Water and wastewater treatment processes generally function best within a pH range of 6 to 8.5. Chemical coagulants and polymers each have an optimum pH where they function best. Fish and most aquatic life do not thrive at pH values lower than 5.

Chapter 2 Essential chemistry concepts

2.6 Acid-base chemistry

- The "p scale" may be used to express other constituents in a solution. In equilibrium chemistry, the concentration of hydroxide may be expressed in terms of pOH, analogous to the pH concept. Mathematically, pOH is deffned as the negative of the logarithm of the hydroxide ion concentration, as shown below.

$$pOH = -\log [OH^-]$$

**Table 2.14** Estimate of pH for several common items.

Item	pH
I M HCl	0
Lemonade	2.2–3.0
Raw apples	2.2–3.0
Milk	6.4–7.6
Pure water	7.0
Drinking water	6.5–8.5
Ammonia	11–12
I M NaOH	14

Chapter 2 Essential chemistry concepts

2.6 Acid-base chemistry

- The conjugate acid(共轭酸) forms when the proton is transferred from the acid to the base; while the conjugate base results from the loss of the proton from the acid. The conjugate acid forms when the proton is transferred from the acid to the base; while the conjugate base (共轭碱) results from the loss of the proton from the acid.

$$HCl_{(aq)} + H_2O_{(l)} \leftrightarrow H_3O^+_{(aq)} + Cl^-_{(aq)}$$
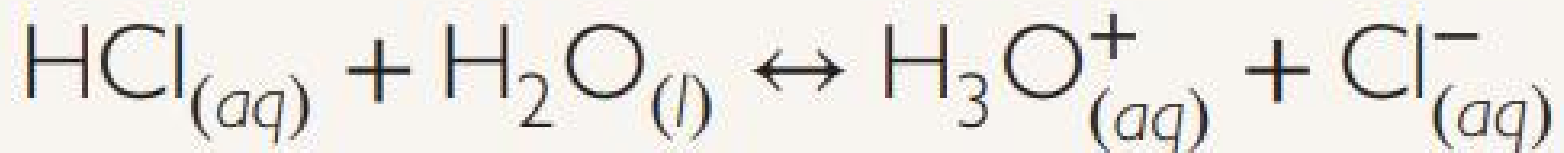
- In the above reaction, hydrochloric acid loses a proton to form chloride, its conjugate base, while water (base) accepts a proton forming the hydronium ion（水合氢离子）, its conjugate acid.

Chapter 2 Essential chemistry concepts

2.6 Acid-base chemistry

2.6.1 Strong acid and base solutions

● Water has the ability to cause many substances to split apart into charged species. This process is known as dissociation(解离) or ionization（电离） . Strong electrolytes （电解质） dissociate completely in water.Almost all salts are completely dissociated in water. Examples of salts that dissociate readily include KBr, NaCl, $CaCl_2$,$Ca(NO_3)_2$, $Fe(ClO_4)_3$, and $Cd(BrO_3)_2$.

● The dissociation of strong acids and bases is almost complete. Few acids are completely dissociated or ionized in water. The dissociation constant of an acid or base is used to quantify its strength. The dissociation constant for an acid is represented by Ka and for a base by Kb. Strong acids have large dissociation constants or ΔG values that are very negative.

● Examples of strong acids (Ka ≈ ∞) include: HCl, HNO_3, H_2SO_4, HBr, HI, and HClO4. Strong bases that dissociate readily (Kb ≈ ∞) include NaOH, KOH, LiOH, and $Ba(OH)_2$.

2.6 Acid-base chemistry

2.6.2 Weak acids and bases

- A weak electrolyte is a compound which does not completely dissociate in water. Most acids and almost all organic acids are weak electrolytes. Examples of weak acids include H_2S, H_2CO_3, HF, H_3PO_4, HCN, and CH_3COOH. Weak bases also result in incomplete dissociation in water. Examples of weak bases include NH_3, N_2H_4 (hydrazine), and organic bases such as $C_6N_5H_2$ (aniline) and $C_2N_5NH_2$ (ethylhyamine).

- Complexes or coordination compounds, which are species of a central metal ion and one or more associated groups are weak electrolytes. Examples of these include: $Ag(NH_3)^+_2$, $Fe(CNS)^{2+}$, $Hg(CN)^+_9$, and $Fe(CN)^{3+}_6$. Water is a weak electrolyte, since it ionizes only slightly into hydrogen and hydroxide ions.

2.6 Acid-base chemistry

2.6.3 pC-pH diagrams

● Graphical techniques that make use of pC-pH diagrams are useful for solving more diffcult acid-base equilibrium problems. The main advantage offered by this technique is that it shows which chemical species are negligible（可忽视的） and which are not. The procedure involves selecting a "master variable" and then drawing curves to show how the concentrations of the various species change as we change the master variable. In acid-base problems, the master variable is $[H^+]$ or pH. On the plot, the log concentration, $\log [C]$, of the various chemical species is plotted versus pH.

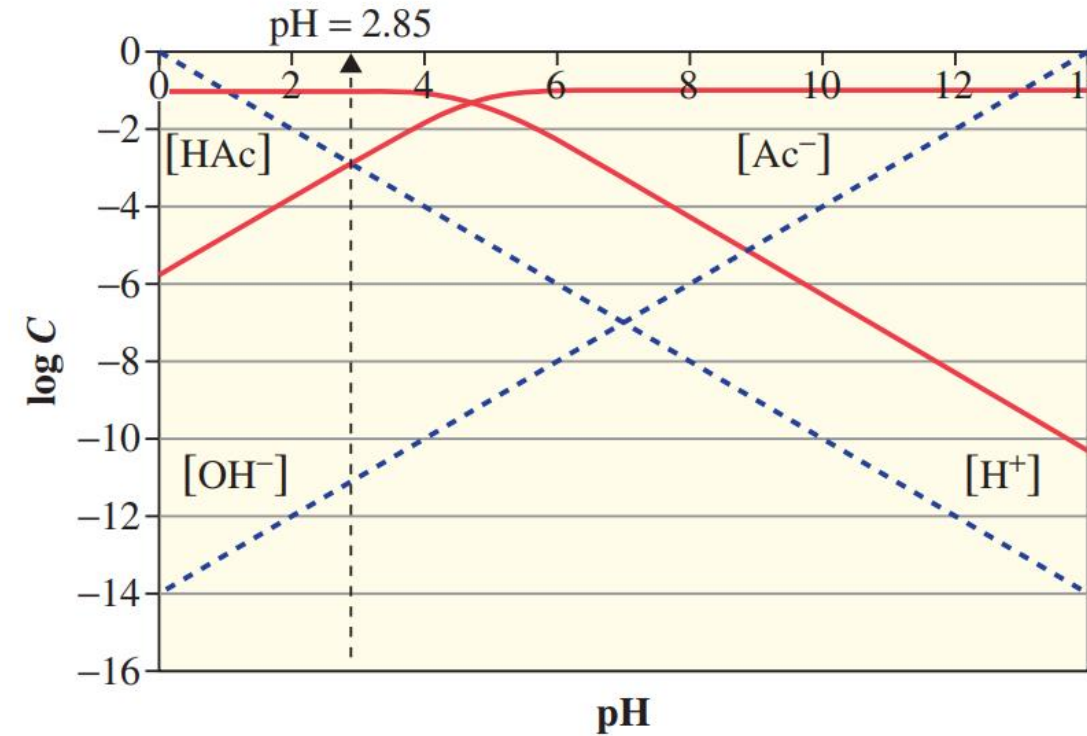**Figure 2.4** pC-pH diagram for 0.1 M acetic acid solution.

2.6 Acid-base chemistry

2.6.4 Buffers

● As previously mentioned, strong acids and bases are considered to dissociate completely or ionize in dilute solutions, while weak acids and bases are only partially ionized. When an acid is added to pure water, the hydrogen ion concentration will increase. Similarly, the hydroxide ion concentration increases when a base is added to pure water.

● Buffers are substances in a solution that resist a change in pH when either an acid or base is added to the solution. Buffered solutions are very important in water chemistry, where we desire to maintain a specific pH. When coagulants are added to raw water to remove turbidity or to precipitate a specific ion, a narrow pH range is necessary for this to occur under optimal conditions. During biological nitrification（硝化反应） in activated sludge systems （活性污泥系统）, both nitrous and nitric acid（亚氮和硝酸） are produced, which can lower the pH of the wastewater, thereby inhibiting the process.

● The final pH of a buffered solution made from a weak acid is dependent upon the ratio of the conjugate base or salt to the acid concentration. The larger the concentration of weak acid, the greater will be the buffering capacity of the solution. In biological systems, phosphoric acid is offen used, since its second pKA value is 7.2.

Chapter 2 Essential chemistry concepts

2.6 Acid-base chemistry

2.6.5 Carbonate system and alkalinity

●The carbonate（碳酸盐） systems is the most important acid-base system in water chemistry, since it serves as the basis of providing natural buffering capacity in water. Alkalinity（碱度） is defined as the buffering capacity of a system to resist a change in pH with the addition of an acid. Alternatively, the buffering capacity of a system to resist a change in pH with the addition of a base is called acidity（酸度）. Traditionally, alkalinity is determined analytically by titrating （滴定）a sample of water with 0.02 N（摩尔浓度） H_2SO_4 to a pH of approximately 4.5. In natural water systems, the total alkalinity of a system is primarily a function of the carbonate system and the hydroxide（氢氧化物） and hydrogen ions.

Chapter 2 Essential chemistry concepts

2.6 Acid-base chemistry

2.6.5 Carbonate system and alkalinity

- Gaseous carbon dioxide, $CO_{2(g)}$
- Aqueous dissolved carbon dioxide, $CO_{2(aq)}$
- Calcium carbonate solids, $CaCO_{3(s)}$

- Bicarbonate, HCO_3^-
- Carbonate, CO_3^{2-}

●The carbonate（碳酸盐） systems is the most important acid-base system in water chemistry, since it serves as the basis of providing natural buffering capacity in water. Alkalinity（碱度） is defined as the buffering capacity of a system to resist a change in pH with the addition of an acid. Alternatively, the buffering capacity of a system to resist a change in pH with the addition of a base is called acidity（酸度）. Traditionally, alkalinity is determined analytically by titrating （滴定）a sample of water with 0.02 N（摩尔浓度） H_2SO_4 to a pH of approximately 4.5. In natural water systems, the total alkalinity of a system is primarily a function of the carbonate system and the hydroxide （氢氧化物） and hydrogen ions.

Chapter 2 Essential chemistry concepts

2.6 Acid-base chemistry

2.6.5 Carbonate system and alkalinity

- Carbon dioxide is an important participant in the carbonate system. It is released into the atmosphere from fossil fuel combustion, volcanoes, biological respiration, and also from supersaturated waters. Autotrophic(自养的) organisms use CO_2 in synthesizing biomass. Atmospheric CO_2 dissolves in water, with the ocean being a major reservoir of aqueous CO_2 in equilibrium with carbonic acid. The concentration of carbonates and bicarbonates（重碳酸盐） in surface and ground waters is highly dependent upon the geological formations and bedrock to which the water is exposed. Regions consisting of dolomite（白云岩） $(CaMg(CO_3)_2)$ or calcite（方解石） $(CaCO_3)$ bedrock will contain high concentrations of carbonate species, including calcium (Ca^{2+}) and magnesium (Mg^{2+}) ions, whereas regions containing igneous rocks（火成岩） will have significantly low levels of these and will exhibit low alkalinity with minimal buffering capacity.

Chapter 2 Essential chemistry concepts

2.7 Solubility (solubility product)

● So far, we have dealt with aqueous solutions in which the chemical species are highly soluble. In this section, our focus will be on liquid-solid species that are partially soluble or insoluble. All solids, no matter how seemingly insoluble, are soluble to some degree. When a solid is placed in water, the ions at the surface of the solid will migrate into the water. This is called dissolution. Simultaneously, ions in the solution will be redeposited on the surface of the solid; this is known as precipitation（淀析）.

● Equilibrium will be reached between the crystals of the compound in the solid state and its ions in solution. In general, the solubility of most compounds increases with increasing temperature.

2.8 Gas phase laws

2.8.1 Boyle's law

● Robert Boyle (1627–1691) conducted experiments with a J-tube to determine the relationship between the pressure of trapped gas and the volume of the gas. Boyle's data indicated that the volume of the gas decreased as the pressure of the gas increased. Stating this another way, volume and pressure are inversely proportional; when one of the parameters increases, the other decreases.

$$P \times V = k_B$$

where:

P = pressure of gas at constant temperature, in of Hg

V = volume of gas at constant temperature, in^3

k_b = Boyle's law constant, in Hg · in^3.

2.8 Gas phase laws

2.8.2 Charles's law

● The French physicist Jacques Charles (1746–1823) showed that the volume of a given amount of gas at constant pressure increases as the temperature of the gases increases. Charles's law may be arranged to show the relationship between the volume and temperature of a given amount of gas at two different measurements.

● Mathematically, Charles's law is stated as follows:

$$V = cT$$

where:

V = volume of gas for a given amount of gas at constant pressure, L

c = Charles's proportionality constant, dimensionless

T = temperature of gas, K.

2.8 Gas phase laws

2.8.3 Avogadro's law

The relationship between the volume of a gas and the number of molecules (6.02×10^{23}) present in the gas at constant pressure and temperature was first postulated by Amadeo Avogadro in 1811. This equation means that the volume of a gas at constant temperature and pressure is directly proportional to the number of moles of gas. Mathematically, this is expressed by the following equation:

$$V = a\,n$$

where:

V = volume of gas at constant pressure and temperature, L

a = Avogadro's proportionality constant, dimensionless

n = number of moles of gas, mol.

Chapter 2 Essential chemistry concepts

2.8 Gas phase laws

2.8.4 Ideal gas law

- Avogadro's, Boyle's, and Charles's laws show how the volume of a gas depends on the number of moles of gas, the pressure, and the temperature. Each of these laws is based on experimental data.

- To solve Equation (2.126), only three of the four parameters are required. According to Zumdahl (2000), the Ideal Gas law is applicable to most gases when the pressure is approximately 1 atm or lower and the temperature is 0° C or higher. Other equations of state must be used at high pressures and lower temperatures.

$$\cancel{V} = n\,a = c\,T = \frac{k_B}{P} \tag{2.123}$$

$$\cancel{V} = \frac{n\,T(a\,c\,k_B)}{P} \tag{2.124}$$

$$\cancel{V} = \frac{n\,T(R)}{P} \tag{2.125}$$

$$P\,\cancel{V} = n\,R\,T \tag{2.126}$$

where:

P = absolute pressure, atm,

$\cancel{V}$ = volume occupied by the gas, L

n = moles of gas,

R = universal gas law constant, $\dfrac{\textbf{0.08206 atm·L}}{\text{mol·K}}$

R = universal gas law constant, $\dfrac{1.986 \text{ cal}}{\text{mol·K}}$,

R = universal gas law constant, $\dfrac{1.986 \text{ BTU}}{\text{lb mol·°R}}$

T = temperature, K ($273.15 + °C$).

2.8 Gas phase laws

2.8.5 Dalton's law

● John Dalton was one of the first scientists to study mixtures of gases. Based on his studies, Dalton stated that, for a mixture of gases in a container, the total pressure exerted is the sum of the partial pressure of each of the gases that are present. Dalton's law is presented mathematically as follows:

The partial pressure of a gas is the pressure that the gas would exert if it were the only gas present in the container, i.e., it is proportional to the percentage by volume of that gas in the mixture.

$$P_T = P_1 + P_2 + P_3 + \ldots + P_i \qquad (2.127)$$

where:

P_i = partial pressure of gaseous component i, atm

P_1, P_2, P_3 = partial pressure of gaseous component 1, 2, and 3, atm

P_T = total pressure of the system, atm.

2.8 Gas phase laws

2.8.6 Raoult's law

- Raoult's Law is a basic principle in physical chemistry that describes the relationship between the vapor pressure of a solvent in a solution and the composition of the solution. The law states that at a given temperature, the vapor pressure of the solvent in a dilute solution is equal to the vapor pressure of the pure solvent multiplied by the molar fraction of the solvent in the solution. Mathematically, Raoult's law is expressed as:

$$P_A = P_A^* x_A \qquad (2.129)$$

where:

P_A^* = vapor pressure of component A, atm

P_A = partial pressure of component A, atm

x_A = mole fraction of component A in the liquid phase.

Chapter 2 Essential chemistry concepts

2.8 Gas phase laws

2.8.6 Raoult's law

- Several organic compounds are very volatile, i.e., they have a high vapor pressure. Volatilization is offen used interchangeably with evaporation in environmental work; it is the transfer of a compound from the liquid phase to the gaseous phase. Table 2.17 lists the vapor pressures of several chemicals as a function of temperature.

Table 2.17 Vapor pressure of several chemical components at specified temperature.

Chemical	Formula	Vapor pressure, kPa	T, °C
Acetone	C_3H_6O	100	55.7
Ammonia	NH_3	100	−33.6
Benzene	C_6H_6	100	79.7
Chloroform	$CHCl_3$	100	60.8
Toluene	C_7H_8	100	110.1
Tetrachloroethylene	C_2Cl_4	100	120.7
Trichloroethylene	C_2HCl_3	100	86.8
2,4,6-Trichlorophenol	$C_6H_3Cl_3O$	100	245.7
Water	H_2O	100	99.6

2.8 Gas phase laws

2.8.6 Raoult's law

- An important application of Raoult's law is in calculations in processes such as distillation and absorption.

- It can be used to predict changes in the vapor pressure and composition of a solution under certain conditions.

- In addition, Raoult's law also helps to understand the deviation of solvent vapor pressure in polymer solutions, which is usually related to the size of solute molecules and the interactions between molecules.

2.8 Gas phase laws

2.8.7 Henry's law

Henry's law describes the relationship between the solubility of a gas in a liquid and the equilibrium pressure of that gas at the liquid surface. It states that at isothermal and isobaric pressure, the solubility of a volatile solute (generally a gas) in a solution is proportional to the equilibrium pressure of the solute at the liquid surface. The mathematical expression of Henry's law is：

$P_g = H \cdot x$,
Where, Pg is the partial pressure of a gas,
H is Henry's constant,
x is the mole fraction of the gas in solution.

2.8 Gas phase laws

2.8.7 Henry's law

- There are several forms of Henry's law, depending on the units associated with the Henry's constant. Henry's law can be expressed to show the relationship between the liquid mole fraction concentration (x_i) of a chemical that is in equilibrium to the gas phase concentration.

- Henry's law generally applies to volatile solutes in dilute solutions and is more accurate when the gas solubility is not high.

- Henry's constant H is a good representation of the amount of gas dissolved, but it is a function of temperature and is independent of pressure. Henry's law is very important in practical applications, such as calculating the solubility of carbon dioxide in the beverage industry.

Chapter 2 Essential chemistry concepts

2.9 Organic chemistry overview

● Organic chemistry is the study of carbon-containing compounds and their properties. Originally, it was believed that organic compounds only could be formed by plants and animals. This was known as the vital-force theory（生命力理论）, and German chemist Friedrich Wohler (1800–1882) disproved this theory when he was able to produce urea, a component of urine(尿素), by heating ammonium cyanate(氰酸铵) according to the following reaction.

● All organic compounds contain carbon in combination with one or more elements. Hydrocarbons consist only of carbon and hydrogen. Many organic compounds contain carbon, hydrogen, and oxygen; yet others contain nitrogen, phosphorus, and sulfur in addition to carbon. Organic compounds are important since they:

  • form the basis for all life;

  • are used in the production of pesticides, herbicides,

  • insecticides, polymers, antibiotics, hormones, and alcohols;

  • cause deleterious effects on the environment, since many of the synthesized organics contain halogens（卤素） and metals which may be toxic and or carcinogenic.

Chapter 2 Essential chemistry concepts

2.9 Organic chemistry overview

● According to Sawyer & McCarty (1994, p. 189), there are seven major differences between organic and inorganic compounds:

• Organics are usually combustible.

• In general, organics have lower boiling and melting points.

•Organics are usually less soluble in water than are inorganics.

• Several organic compounds may exist for a given formula; this is known as isomerism（同分异构）.

• Chemical reactions involving organic compounds are often quite slow, since these reactions are molecular rather than ionic.

• Organic compounds have high molecular weights, often greater than 1,000.

• Most organic compounds can serve as an energy and carbon source for bacteria and other microorganisms.

Chapter 2 Essential chemistry concepts

2.9 Organic chemistry overview

●There are three major types of organic compounds:aliphatic（脂肪族）, aromatic（芳香族） and heterocyclic（杂环族）:

• Aliphatic organic compounds (open-chain structures) contain carbon-carbon bonds with functional groups linked to a straight or branched chain.

• Aromatic organics consist of six-member carbon ring structures that contain double bonds rather than single-covalent bonds.

• Finally, the heterocyclic organic compounds are those that have a ring structure in which at least one element is other than carbon.

Chapter 2 Essential chemistry concepts

2.9 Organic chemistry overview

2.9.1 Introduction to hydrocarbons (alkanes, alkenes, and alkynes烷烃、烯烃、炔)

● Hydrocarbons consist only of hydrogen and carbon, and they may be saturated or unsaturated. A saturated hydrocarbon means that adjacent carbon atoms are joined together by a single covalent bond and all other bonds are made with hydrogen. They are represented by the following formula: $CnH2n+2$. Alkanes are also called the paraffins（石蜡） or aliphatic hydrocarbons.
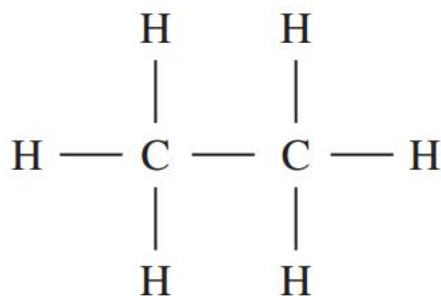
Figure 2.9 Structural formula of the saturated hydrocarbon ethane.

Table 2.19 Formulas of the first ten straight-chain alkanes or paraffins.

Name	Formula	Structure	BP, °C	MP, °C
Methane	CH_4	CH_4	−161.5	−183
Ethane	C_2H_6	CH_3CH_3	−88.3	−172
Propane	C_3H_8	$CH_3CH_2CH_3$	−42.2	−187.1
Butane	C_4H_{10}	$CH_3CH_2CH_2CH_3$	−0.6	−135
Pentane	C_5H_{12}	$CH_3CH_2CH_2CH_2CH_3$	36.2	−130
Hexane	C_6H_{14}	$CH_3CH_2CH_2CH_2CH_2CH_3$	69.0	−94.3
Heptane	C_7H_{16}	$CH_3CH_2CH_2CH_2CH_2CH_2CH_3$	98.5	−90.5
Octane	C_8H_{18}	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	125.8	−56.5
Nonane	C_9H_{20}	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	150.7	−53.7
Decane	$C_{10}H_{22}$	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	174	−30

Chapter 2 Essential chemistry concepts

2.9 Organic chemistry overview

2.9.1 Introduction to hydrocarbons (alkanes, alkenes, and alkynes烷烃、烯烃、炔)

● Unsaturated hydrocarbons are those that have at least two carbon atoms that are joined together by more than a single covalent bond; the remaining bonds are formed with hydrogen, i.e., they contain double and triple bonds. Alkenes are hydrocarbons that contain at least one double bond and are represented by the following formula: $CnH2n$. They are also called olefins（烯烃）, and their names all end with the suffix –ene.
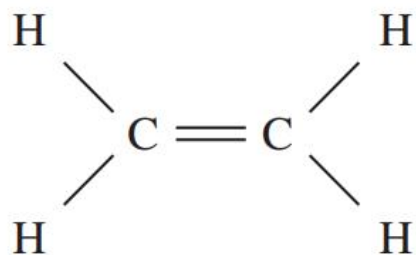
Figure 2.10 Structural formula of the unsaturated hydrocarbon ethylene.

Table 2.20 Formulas of selected alkenes.

Name	Formula	Structure	BP, °C	MP, °C
Ethene	C_2H_4	C_2H_4	−103.9**	−169.4**
Propene	C_3H_6	$CH_2 = CHCH_3$	−47*	−185*
1−Butene	C_4H_8	$CH_2 = CHCH_2CH_3$	−6.5*	−130*
2−Methylpropene	C_4H_8	$(CH_3)_2C = CH_2$	−6.9*	−141*
1−Pentene	C_5H_{10}	$CH_2 = CH(CH_2)_2CH_3$	30*	−138*
1−Hexene	C_6H_{12}	$CH_2 = CH(CH_2)_3CH_3$	64.1**	−98.5**
2−Methyl−2−pentene	C_6H_{12}	$CH_3CH_2CH = C(CH_3)_2$	67−69***	−135***
1−Heptene	C_7H_{14}	$CH_2 = CH(CH_2)_4CH_3$	95**	−120**
2,4−Dimethyl−2−pentene	C_7H_{14}	$(CH_3)_2CHC(CH_3) = CHCH_3$	83****	−128****

Chapter 2 Essential chemistry concepts

2.9 Organic chemistry overview

2.9.1 Introduction to hydrocarbons (alkanes, alkenes, and alkynes烷烃、烯烃、炔)

● Alkynes are hydrocarbons that contain at least one triple bond and are represented by the following formula: CnHn. They are also called olefins（烯烃）, and their names all end with the suffix, –yne.

Table 2.21 Formulas of selected alkynes.

Name	Formula	BP, °C	MP, °C
Ethyne	H−C≡C−H	−84.7 sp	−80.8 (triple point)
Propyne	CH_3 − C≡C−H	−23.2	−102.7
1−Butyne	CH_3CH_2−C≡C−H	8.08	−125.7
2−Butyne	CH_3−C≡C−CH_3	26.9	−32.2
1−Pentyne	$CH_3CH_2CH_2$−C≡C−H	40.1	−90
2−Pentyne	CH_3CH_2−C≡C−CH_3	56.1	−109.3

2.9 Organic chemistry overview

2.9.1 Introduction to hydrocarbons (alkanes, alkenes, and alkynes烷烃、烯烃、炔)

● Halogenated hydrocarbons（卤代烃）, such as those involving the substitution of a hydrogen atom with a chlorine molecule to alkanes and alkenes, include several commercial products used as solvents, refrigerants, lubricants（润滑剂）, hydraulic fluids（液压油）, aerosol propellants（气溶胶推进剂）, polymers（聚合物）, and pesticides .

2.9 Organic chemistry overview

2.9.2 Aromatic hydrocarbons（芳香烃）

● An aromatic hydrocarbon, or arene or aryl hydrocarbon（芳烃）, is a hydrocarbon that contains alternating single and double bonds between carbons. The aromatic organic carbons all contain a six-membered ring of carbon atoms called the benzene ring.

● Benzene has the formula C6H6 and is the simplest of the aromatic hydrocarbons.

● Some of the aromatic hydrocarbons have pleasant odors: cinnamon, vanillin, and wintergreen are examples.Aromatic compounds are important to industry and living systems. Chemicals and polymers such as styrene（苯乙烯）, phenol（苯酚）.
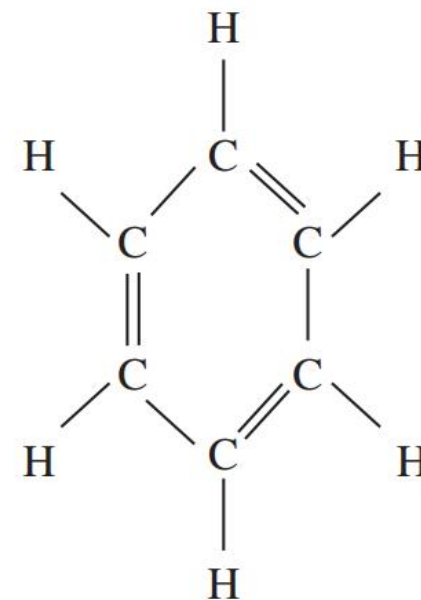
Figure 2.11 Lewis structure for benzene ring.

2.9 Organic chemistry overview

2.9.2 Aromatic hydrocarbons（芳香烃）

● Other aromatics such as histidine, phenylalanine, tryptophan, and tyrosine(组氨酸、苯丙氨酸、色氨酸和酪氨酸), serve as basic building blocks of proteins. The genetic code of all organisms, DNA and RNA, consists of adenine, thymine, cytosine, guanine, and uracil, which are aromatic purines or pyrimidines.

● Benzene, toluene, ethyl benzene, and xylene (苯、甲苯、乙苯和二甲苯)collectively referred to as BTEX is commonly found at contaminated sites.They are associated with petroleum products and offen enter the environment from leaking underground storage tanks (LUSTs).
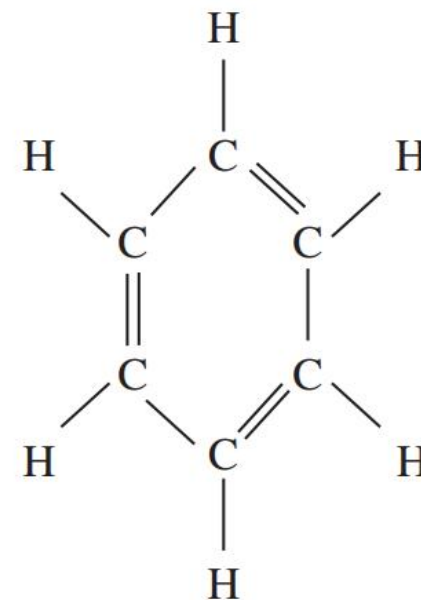
Figure 2.11 Lewis structure for benzene ring.

Chapter 2 Essential chemistry concepts

2.9 Organic chemistry overview

2.9.3 Heterocyclic organic compounds

● Heterocyclic organic compounds have at least one other element in their ring structure other than carbon. These compounds may be either aliphatic or aromatic in nature. Most of the heterocyclic organic compounds in environmental engineering relate to biological processes, i.e., synthesis and other biochemical reactions. Some six-membered aromatic heterocyclic compounds are: purine, pyrimidine, adenine, guanine, cytosine, uracil, and thymine.These compounds are important in the synthesis of proteins and deoxyribonucleic acid (DNA).

2.9.4 Functional groups(官能团) of environmental importance

● As previously mentioned, organic compounds generally contain hydrogen, oxygen, nitrogen, sulfur, and other elements in addition to carbon. The vast array of organic compounds that exist are actually hydrocarbon derivatives that contain additional atoms or groups of atoms called functional groups.

● Alcohols（醇） are characterized by the presence of the hydroxide group (−OH). When alcohols react with a strong acid, they act as bases, i.e., accept protons. The simplest aromatic alcohol is phenol (苯酚)which has a hydroxide group attached to the benzene ring. In general, phenols are more acidic than alcohols and water. Aldehydes（醛）and ketones（酮） contain the carbonyl group (C = O)羟基. Compounds containing the −COOH group are weak acids (carboxylic acids羧酸). Esters（酯） are derived from carboxylic acids.

● Amines(胺) are considered derivatives(衍生物) of ammonia with one, two, or three hydrogen atoms replaced by an alkyl group（烷基）. The amines resemble ammonia and act as weak bases. Amides（酰胺） may be produced from ammonia and carboxylic acids.

Chapter 2 Essential chemistry concepts

Summary:

• Environmental engineers must have a ffrm foundation in chemical concepts, because these are applied to various treatment systems when dealing with water, wastewater, residuals, and air pollution problems.

• A dimension is a physical quantity expressing length, time, temperature, pressure, velocity, and weight. It must be accompanied by the appropriate set of units to quantify the dimension.

•The concentration of a substance in a solution can be expressed in a number of ways.

•In environmental engineering, the flow rate may be given either on a mass or volumetric basis.

Detention time (??) is a fundamental concept in environmental engineering and it represents the average unit of time that a fluid particle remains in the system. Detention time is calculated by dividing the volume of the tank or container by the volumetric ffow rate.

• Engineers must make sure that all chemical equations are properly balanced before using to calculate chemical dosages and quantities.

• In oxidation-reduction or redox reactions, electrons are transferred and the oxidation number of a chemical species changes.

•Thermodynamics allows engineers and chemists to predict whether or not a chemical reaction will proceed as written. It does not allow one to determine the rate at which a reaction takes place.

Summary:

• The equilibrium constant (K) can be determined from free energy data. It can be used to determine the concentration of various chemical species at equilibrium.

• Acids are proton donors and bases accept protons.

• Acid-base chemistry involves estimating the concentration of various chemical entities and pH when either an acid or base is added to a solution.

• The carbonate system is the most important natural buffering system encountered in environmental engineering. It is directly related to alkalinity, which is defined as the buffering capacity of a water to resist a change in pH when an acid is added.

• Liquid-solid species that are partially soluble or insoluble can be explained using the solubility product (Ksp). TTe solubility of most substances increases with temperature;

• Proper application of gas phase laws is essential for designing gas transfer systems, gas strippers, determining saturation concentration of dissolved gases in aqueous solutions, and understanding the relationship between pressure and volume of a gas and between temperature and volume of a gas.

• Organic chemistry is the study of carbon-containing compounds and their properties. Organic compounds are important because: they form the basis of all life; they are used in the production of pesticides, herbicides, insecticides, polymers, antibiotics, hormones, and alcohols; and they cause detrimental affects to the environment, since many of them are toxic and/or carcinogenic.

Thanks!