

WU CHEM 199 BETTER LIVING THROUGH CHEMISTRY



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Chemistry 199:

Better Living Through Chemistry

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CHAPTER OVERVIEW

1: Chemicals in Food

The first of our four topics is about the food we eat. This topic starts with a brief introduction to interpreting chemical structures of organic molecules, which leads into looking at the main macro-nutrients (carbohydrates, proteins and fats) that we take in and how we use them for energy, as well as the micro-nutrients (vitamins and minerals) we ingest and what purpose they serve.

1.1: What are chemicals?

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1.1: What are chemicals?

Chemicals are all around us in different forms: the food we eat, the water we drink, and pharmaceuticals we design to have particular effects on our bodies. The first section starts with a brief review of what chemicals are, and then looks at how we can divide up chemicals by type: organic and inorganic.

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1.1.1: Solids, Liquids, and Gases

Learning Objectives

- Describe the different states of matter.
- Describe the different changes that occur between solid, liquid, and gas.

Matter can exist in one of several different states, including a gas, liquid, or solid state. The amount of energy in molecules of matter determines the **state of matter**.

- A **gas** is a state of matter in which atoms or molecules have enough energy to move freely. The molecules come into contact with one another only when they randomly collide.
- A **liquid** is a state of matter in which atoms or molecules are constantly in contact but have enough energy to keep changing positions relative to one another.
- A **solid** is a state of matter in which atoms or molecules do not have enough energy to move. They are constantly in contact and in fixed positions relative to one another.

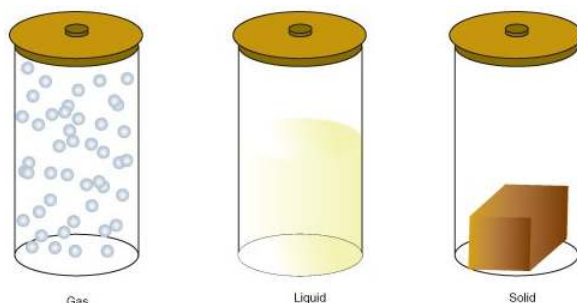
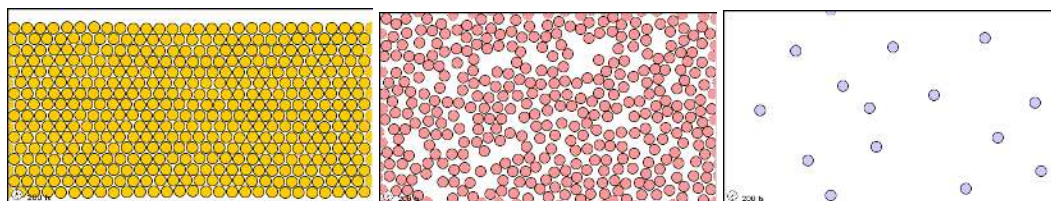


Figure 1.1.1.1: States of Matter. All three containers contain a substance with the same mass, but the substances are in different states. In the left-hand container, the substance is a gas, which has spread to fill its container. It takes both the shape and volume of the container. In the middle container, the substance is a liquid, which has spread to take the shape of its container but not the volume. In the right-hand container, the substance is a solid, which takes neither the shape nor the volume of its container.

In Figure 1.1.1.2 all three phases are shown at the submicroscopic level in animations. Notice how the movement and freedom of molecules steadily increases as attractive forces decrease from solid to liquid to gas phase.



SOLID LIQUID GAS

Figure 1.1.1.2 Animation of all three phases at the submicroscopic level.

The change from solid to liquid usually does not significantly change the volume of a substance. However, the change from a liquid to a gas significantly increases the volume of a substance, by a factor of 1,000 or more. Figures 1.1.1.3 and 1.1.1.4 show the differences among solids, liquids, and gases at the molecular level, while Table 1.1.1.1 lists the different characteristics of these states.

Table 1.1.1.1 Characteristics of the Three States of Matter

Characteristic	Solid	Liquid	Gas
shape	definite	indefinite	indefinite
volume	definite	definite	indefinite
relative intermolecular interaction strength	strong	moderate	weak

Characteristic	Solid	Liquid	Gas
relative particle positions	in contact and fixed in place	in contact but not fixed	not in contact, random positions

✓ Example 1.1.1.1

What state or states of matter does each statement, describe?

- This state has a definite volume.
- This state has no definite shape.
- This state allows the individual particles to move about while remaining in contact.

Solution

- This statement describes either the liquid state or the solid state.
- This statement describes either the liquid state or the gas state.
- This statement describes the liquid state.

? Exercise 1.1.1.1

What state or states of matter does each statement describe?

- This state has individual particles in a fixed position with regard to each other.
- This state has individual particles far apart from each other in space.
- This state has indefinite shape.

Answer a

solid

Answer b

gas

Answer c

liquid or gas

Phase Changes

A phase change is a physical process in which a substance goes from one phase to another. Usually the change occurs when adding or removing heat at a particular temperature, known as the melting point or the boiling point of the substance. The **melting point** is the temperature at which the substance goes from a solid to a liquid (or from a liquid to a solid). The **boiling point** is the temperature at which a substance goes from a liquid to a gas (or from a gas to a liquid). The nature of the phase change depends on the direction of the heat transfer. Heat going *into* a substance changes it from a solid to a liquid or a liquid to a gas. Removing heat *from* a substance changes a gas to a liquid or a liquid to a solid.

Two key points are worth emphasizing. First, at a substance's melting point or boiling point, two phases can exist simultaneously. Take water (H_2O) as an example. On the Celsius scale, H_2O has a melting point of 0°C and a boiling point of 100°C . At 0°C , both the solid and liquid phases of H_2O can coexist. However, if heat is added, some of the solid H_2O will melt and turn into liquid H_2O . If heat is removed, the opposite happens: some of the liquid H_2O turns into solid H_2O . A similar process can occur at 100°C : adding heat increases the amount of gaseous H_2O , while removing heat increases the amount of liquid H_2O (Figure 1.1.1.3).

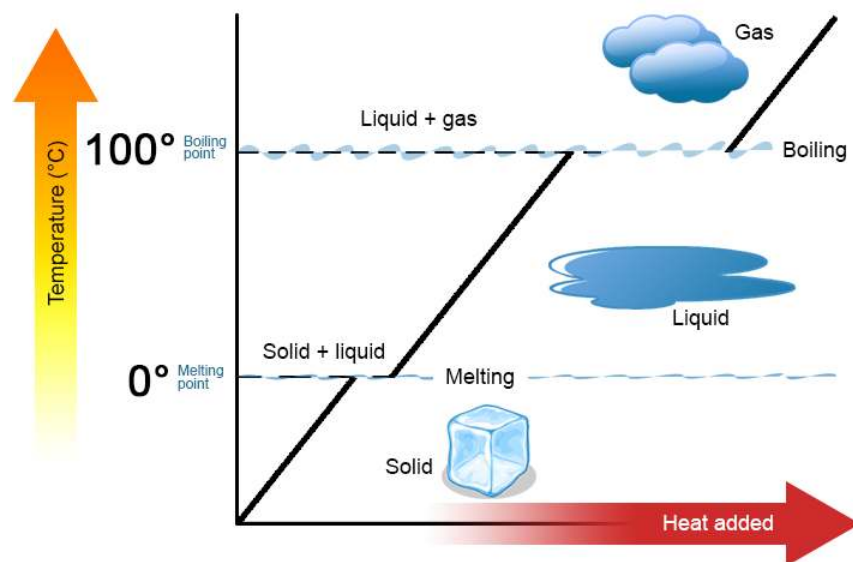


Figure 1.1.1.3: Heating curve for water. As heat is added to solid water, the temperature increases until it reaches 0 °C, the *melting point*. At this point, the *phase change*, added heat goes into changing the state from a solid to liquid. Only when this phase change is complete, the temperature can increase. (CC BY 3.0 Unported; Community College Consortium for Bioscience Credentials).

Water is a good substance to use as an example because many people are already familiar with it. Other substances have melting points and boiling points as well.

Second, as shown in Figure 1.1.1.3 **the temperature of a substance does not change** as the substance goes **from one phase to another**. In other words, phase changes are isothermal (isothermal means “constant temperature”). Again, consider H₂O as an example. Solid water (ice) can exist at 0°C. If heat is added to ice at 0°C, some of the solid changes phase to make liquid, which is also at 0°C. Remember, the solid and liquid phases of H₂O can coexist at 0°C. Only after all of the solid has melted into liquid does the addition of heat change the temperature of the substance.

Summary of Phase Changes

All of the changes of state that occur between solid, liquid, and gas are summarized in the diagram in the figure below. **Freezing** is the opposite of melting, and both represent the equilibrium between the solid and liquid states. **Evaporation** occurs when a liquid turns to a gas. **Condensation** is the opposite of vaporization, and both represent the equilibrium between the liquid and gas states. **Deposition** is the opposite of sublimation, and both represent the equilibrium between the solid and gas states.

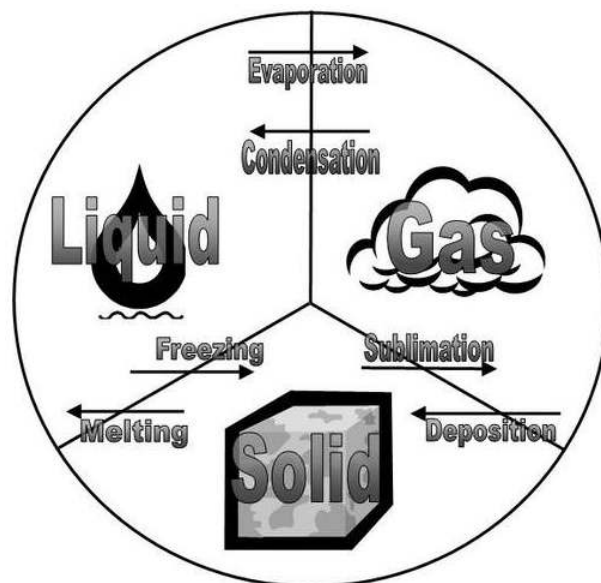


Figure 1.1.1.4: Solid, liquid, and gas states with the terms for each change of state that occurs between them.

Liquid evaporates into gas in freezes into a solid; gas condenses into a liquid depositions into a solid; solids melt into a liquid and sublimation into a gas

Summary

- Solids, liquids, and gases are different phases that have their own unique properties.
- A change of state (or phase change) can be brought about by putting heat into a system or removing it from the system.

Contributors and Attributions

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1.1.2: Molecules and Molecular Compounds

Learning Objectives

- to understand the differences between covalent and ionic bonding.

The atoms in all substances that contain multiple atoms are held together by electrostatic interactions—interactions between electrically charged particles such as protons and electrons. Electrostatic attraction between oppositely charged species (positive and negative) results in a force that causes them to move toward each other, like the attraction between opposite poles of two magnets. In contrast, electrostatic repulsion between two species with the same charge (either both positive or both negative) results in a force that causes them to repel each other, as do the same poles of two magnets. Atoms form chemical compounds when the attractive electrostatic interactions between them are stronger than the repulsive interactions. Collectively, the attractive interactions between atoms are called chemical bonds.

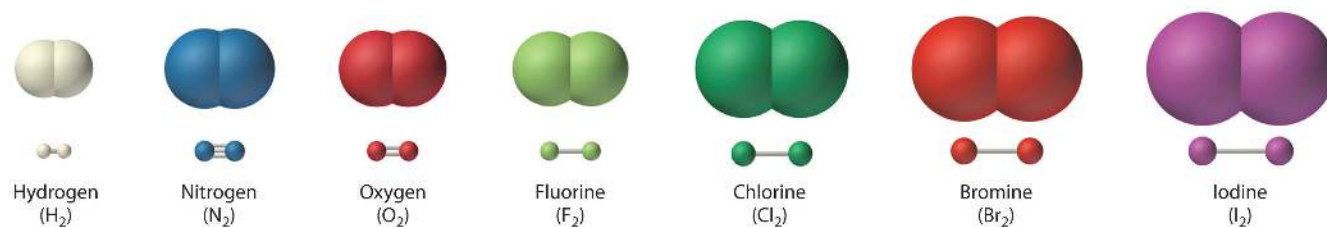
Chemical bonds are generally divided into two fundamentally different types: ionic and covalent. In reality, however, the bonds in most substances are neither purely ionic nor purely covalent, but lie on a spectrum between these extremes. Although purely ionic and purely covalent bonds represent extreme cases that are seldom encountered in any but very simple substances, a brief discussion of these two extremes helps explain why substances with different kinds of chemical bonds have very different properties. Ionic compounds consist of positively and negatively charged ions held together by strong electrostatic forces, whereas covalent compounds generally consist of molecules, which are groups of atoms in which one or more pairs of electrons are shared between bonded atoms. In a covalent bond, atoms are held together by the electrostatic attraction between the positively charged nuclei of the bonded atoms and the negatively charged electrons they share. This discussion of structures and formulas begins by describing covalent compounds. The energetic factors involved in bond formation are described in more quantitative detail in later.

Ionic compounds consist of ions of opposite charges held together by strong electrostatic forces, whereas pairs of electrons are shared between bonded atoms in covalent compounds.

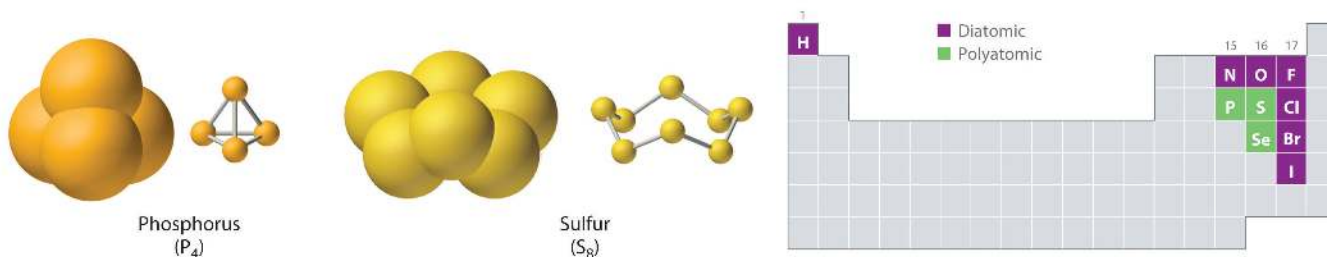
Covalent Molecules and Compounds

Just as an atom is the simplest unit that has the fundamental chemical properties of an element, a molecule is the simplest unit that has the fundamental chemical properties of a covalent compound. Some pure elements exist as covalent molecules. Hydrogen, nitrogen, oxygen, and the halogens occur naturally as the diatomic (“two atoms”) molecules H_2 , N_2 , O_2 , F_2 , Cl_2 , Br_2 , and I_2 (part (a) in Figure 1.1.2.1). Similarly, a few pure elements exist as polyatomic (“many atoms”) molecules, such as elemental phosphorus and sulfur, which occur as P_4 and S_8 (part (b) in Figure 1.1.2.1).

Each covalent compound is represented by a molecular formula, which gives the atomic symbol for each component element, in a prescribed order, accompanied by a subscript indicating the number of atoms of that element in the molecule. The subscript is written only if the number of atoms is greater than 1. For example, water, with two hydrogen atoms and one oxygen atom per molecule, is written as H_2O . Similarly, carbon dioxide, which contains one carbon atom and two oxygen atoms in each molecule, is written as CO_2 .



(a) Elements that exist as diatomic molecules



(b) Elements that exist as polyatomic molecules

Figure 1.1.2.1: Elements That Exist as Covalent Molecules. (a) Several elements naturally exist as diatomic molecules, in which two atoms (E) are joined by one or more covalent bonds to form a molecule with the general formula E_2 . (b) A few elements naturally exist as polyatomic molecules, which contain more than two atoms. For example, phosphorus exists as P_4 tetrahedra—regular polyhedra with four triangular sides—with a phosphorus atom at each vertex. Elemental sulfur consists of a puckered ring of eight sulfur atoms connected by single bonds. Selenium is not shown due to the complexity of its structure.

A: Elements that exist as diatomic molecules: H_2 , N_2 , O_2 , F_2 , Cl_2 , Br_2 , and I_2 . B: Elements that exist as polyatomic molecules: P_4 and S_8 .

Covalent compounds that predominantly contain carbon and hydrogen are called organic compounds. The convention for representing the formulas of organic compounds is to write carbon first, followed by hydrogen and then any other elements in alphabetical order (e.g., CH_4O is methyl alcohol, a fuel). Compounds that consist primarily of elements other than carbon and hydrogen are called inorganic compounds; they include both covalent and ionic compounds. In inorganic compounds, the component elements are listed beginning with the one farthest to the left in the periodic table, as in CO_2 or SF_6 . Those in the same group are listed beginning with the lower element and working up, as in ClF . By convention, however, when an inorganic compound contains both hydrogen and an element from groups 13–15, hydrogen is usually listed last in the formula. Examples are ammonia (NH_3) and silane (SiH_4). Compounds such as water, whose compositions were established long before this convention was adopted, are always written with hydrogen first: Water is always written as H_2O , not OH_2 . The conventions for inorganic acids, such as hydrochloric acid (HCl) and sulfuric acid (H_2SO_4), are described in Section 2.8.

For organic compounds: write C first, then H, and then the other elements in alphabetical order. For molecular inorganic compounds: start with the element at far left in the periodic table; list elements in same group beginning with the lower element and working up.

✓ Example 1.1.2.1

Write the molecular formula of each compound.

- The phosphorus-sulfur compound that is responsible for the ignition of so-called strike anywhere matches has 4 phosphorus atoms and 3 sulfur atoms per molecule.
- Ethyl alcohol, the alcohol of alcoholic beverages, has 1 oxygen atom, 2 carbon atoms, and 6 hydrogen atoms per molecule.
- Freon-11, once widely used in automobile air conditioners and implicated in damage to the ozone layer, has 1 carbon atom, 3 chlorine atoms, and 1 fluorine atom per molecule.

Given: identity of elements present and number of atoms of each

Asked for: molecular formula

Strategy:

- Identify the symbol for each element in the molecule. Then identify the substance as either an organic compound or an inorganic compound.
- If the substance is an organic compound, arrange the elements in order beginning with carbon and hydrogen and then list the other elements alphabetically. If it is an inorganic compound, list the elements beginning with the one farthest left in the periodic table. List elements in the same group starting with the lower element and working up.
- From the information given, add a subscript for each kind of atom to write the molecular formula.

Solution

a

- The molecule has 4 phosphorus atoms and 3 sulfur atoms. Because the compound does not contain mostly carbon and hydrogen, it is inorganic.
- Phosphorus is in group 15, and sulfur is in group 16. Because phosphorus is to the left of sulfur, it is written first.
- Writing the number of each kind of atom as a right-hand subscript gives P_4S_3 as the molecular formula.

b.

- Ethyl alcohol contains predominantly carbon and hydrogen, so it is an organic compound.
- The formula for an organic compound is written with the number of carbon atoms first, the number of hydrogen atoms next, and the other atoms in alphabetical order: CHO.
- Adding subscripts gives the molecular formula C_2H_6O .

c

- Freon-11 contains carbon, chlorine, and fluorine. It can be viewed as either an inorganic compound or an organic compound (in which fluorine has replaced hydrogen). The formula for Freon-11 can therefore be written using either of the two conventions.
- According to the convention for inorganic compounds, carbon is written first because it is farther left in the periodic table. Fluorine and chlorine are in the same group, so they are listed beginning with the lower element and working up: CClF. Adding subscripts gives the molecular formula CCl_3F .
- We obtain the same formula for Freon-11 using the convention for organic compounds. The number of carbon atoms is written first, followed by the number of hydrogen atoms (zero) and then the other elements in alphabetical order, also giving CCl_3F .

? Exercise 1.1.2.1

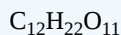
Write the molecular formula for each compound.

- Nitrous oxide, also called “laughing gas,” has 2 nitrogen atoms and 1 oxygen atom per molecule. Nitrous oxide is used as a mild anesthetic for minor surgery and as the propellant in cans of whipped cream.
- Sucrose, also known as cane sugar, has 12 carbon atoms, 11 oxygen atoms, and 22 hydrogen atoms.
- Sulfur hexafluoride, a gas used to pressurize “unpressurized” tennis balls and as a coolant in nuclear reactors, has 6 fluorine atoms and 1 sulfur atom per molecule.

Answer a



Answer b



Answer c



Representations of Molecular Structures

Molecular formulas give only the elemental composition of molecules. In contrast, structural formulas show which atoms are bonded to one another and, in some cases, the approximate arrangement of the atoms in space. Knowing the structural formula of a

compound enables chemists to create a three-dimensional model, which provides information about how that compound will behave physically and chemically.

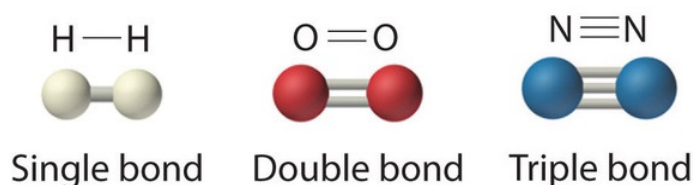


Figure 1.1.2.2: Molecules That Contain Single, Double, and Triple Bonds. Hydrogen (H_2) has a single bond between atoms. Oxygen (O_2) has a double bond between atoms, indicated by two lines ($=$). Nitrogen (N_2) has a triple bond between atoms, indicated by three lines ($\equiv$). Each bond represents an electron pair.

The structural formula for H_2 can be drawn as $\text{H}-\text{H}$ and that for I_2 as $\text{I}-\text{I}$, where the line indicates a single pair of shared electrons, a single bond. Two pairs of electrons are shared in a double bond, which is indicated by two lines—for example, O_2 is $\text{O}=\text{O}$. Three electron pairs are shared in a triple bond, which is indicated by three lines—for example, N_2 is $\text{N}\equiv\text{N}$ (see Figure 1.1.2.2). Carbon is unique in the extent to which it forms single, double, and triple bonds to itself and other elements. The number of bonds formed by an atom in its covalent compounds is not arbitrary. Hydrogen, oxygen, nitrogen, and carbon have very strong tendencies to form substances in which they have one, two, three, and four bonds to other atoms, respectively (Table 1.1.2.1).

Table 1.1.2.1: The Number of Bonds That Selected Atoms Commonly Form to Other Atoms

Atom	Number of Bonds
H (group 1)	1
O (group 16)	2
N (group 15)	3
C (group 14)	4

The structural formula for water can be drawn as follows:



Because the latter approximates the experimentally determined shape of the water molecule, it is more informative. Similarly, ammonia (NH_3) and methane (CH_4) are often written as planar molecules:

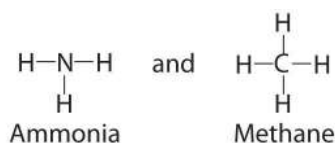


Figure 1.1.2.3, is tetrahedral: the hydrogen atoms are positioned at every other vertex of a cube. Many compounds—carbon compounds, in particular—have four bonded atoms arranged around a central atom to form a tetrahedron.

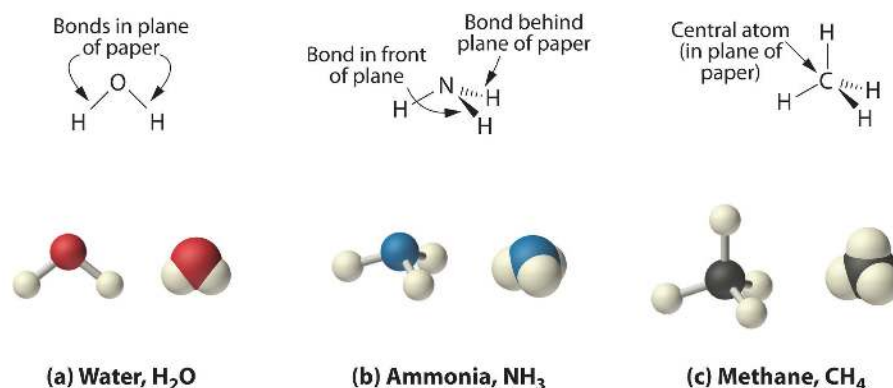
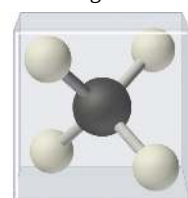


Figure 1.1.2.3: The Three-Dimensional Structures of Water, Ammonia, and Methane. (a) Water is a V-shaped molecule, in which all three atoms lie in a plane. (b) In contrast, ammonia has a pyramidal structure, in which the three hydrogen atoms form the base of the pyramid and the nitrogen atom is at the vertex. (c) The four hydrogen atoms of methane form a tetrahedron; the carbon atom lies in the center.

A: Bent configuration of H_2O . B: Trigonal pyramidal configuration of ammonia. C: Tetrahedral configuration of methane.



Tetrahedral structure of methane, CH_4

Methane CH_4 has a three-dimensional, tetrahedral structure.

Figures 1.1.2.1, 1.1.2.2 and 1.1.2.3 illustrate different ways to represent the structures of molecules. It should be clear that there is no single “best” way to draw the structure of a molecule; the method used depends on which aspect of the structure should be emphasized and how much time and effort is required. Figure 1.1.2.4 shows some of the different ways to portray the structure of a slightly more complex molecule: methanol. These representations differ greatly in their information content. For example, the molecular formula for methanol (Figure 1.1.2.4a) gives only the number of each kind of atom; writing methanol as CH_4O tells nothing about its structure. In contrast, the structural formula (Figure 1.1.2.4b) indicates how the atoms are connected, but it makes methanol look as if it is planar (which it is not). Both the ball-and-stick model (part (c) in Figure 1.1.2.4) and the perspective drawing (Figure 1.1.2.4d) show the three-dimensional structure of the molecule. The latter (also called a wedge-and-dash representation) is the easiest way to sketch the structure of a molecule in three dimensions. It shows which atoms are above and below the plane of the paper by using wedges and dashes, respectively; the central atom is always assumed to be in the plane of the paper. The space-filling model (part (e) in Figure 1.1.2.4) illustrates the approximate relative sizes of the atoms in the molecule, but it does not show the bonds between the atoms. In addition, in a space-filling model, atoms at the “front” of the molecule may obscure atoms at the “back.”

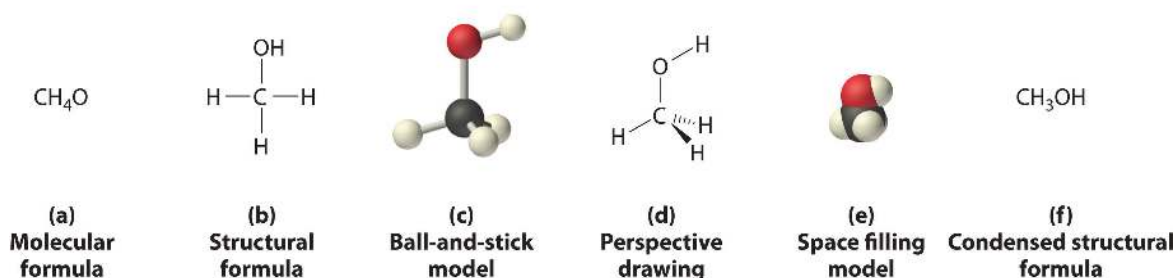


Figure 1.1.2.4: Different Ways of Representing the Structure of a Molecule. (a) The molecular formula for methanol gives only the number of each kind of atom present. (b) The structural formula shows which atoms are connected. (c) The ball-and-stick model shows the atoms as spheres and the bonds as sticks. (d) A perspective drawing (also called a wedge-and-dash representation) attempts to show the three-dimensional structure of the molecule. (e) The space-filling model shows the atoms in the molecule but not the bonds. (f) The condensed structural formula is by far the easiest and most common way to represent a molecule.

Although a structural formula, a ball-and-stick model, a perspective drawing, and a space-filling model provide a significant amount of information about the structure of a molecule, each requires time and effort. Consequently, chemists often use a condensed structural formula (part (f) in Figure 1.1.2.4), which omits the lines representing bonds between atoms and simply lists the atoms bonded to a given atom next to it. Multiple groups attached to the same atom are shown in parentheses, followed by a subscript that indicates the number of such groups. For example, the condensed structural formula for methanol is CH_3OH , which indicates that the molecule contains a CH_3 unit that looks like a fragment of methane (CH_4). Methanol can therefore be viewed either as a methane molecule in which one hydrogen atom has been replaced by an $-\text{OH}$ group or as a water molecule in which one hydrogen atom has been replaced by a $-\text{CH}_3$ fragment. Because of their ease of use and information content, we use condensed structural formulas for molecules throughout this text. Ball-and-stick models are used when needed to illustrate the three-dimensional structure of molecules, and space-filling models are used only when it is necessary to visualize the relative sizes of atoms or molecules to understand an important point.

✓ Example 1.1.2.2: Molecular Formulas

Write the molecular formula for each compound. The condensed structural formula is given.

- Sulfur monochloride (also called disulfur dichloride) is a vile-smelling, corrosive yellow liquid used in the production of synthetic rubber. Its condensed structural formula is ClSSCl .
- Ethylene glycol is the major ingredient in antifreeze. Its condensed structural formula is $\text{HOCH}_2\text{CH}_2\text{OH}$.
- Trimethylamine is one of the substances responsible for the smell of spoiled fish. Its condensed structural formula is $(\text{CH}_3)_3\text{N}$.

Given: condensed structural formula

Asked for: molecular formula

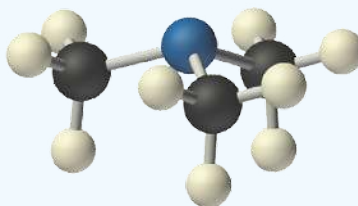
Strategy:

- Identify every element in the condensed structural formula and then determine whether the compound is organic or inorganic.
- As appropriate, use either organic or inorganic convention to list the elements. Then add appropriate subscripts to indicate the number of atoms of each element present in the molecular formula.

Solution:

The molecular formula lists the elements in the molecule and the number of atoms of each.

- A** Each molecule of sulfur monochloride has two sulfur atoms and two chlorine atoms. Because it does not contain mostly carbon and hydrogen, it is an inorganic compound. **B** Sulfur lies to the left of chlorine in the periodic table, so it is written first in the formula. Adding subscripts gives the molecular formula S_2Cl_2 .
- A** Counting the atoms in ethylene glycol, we get six hydrogen atoms, two carbon atoms, and two oxygen atoms per molecule. The compound consists mostly of carbon and hydrogen atoms, so it is organic. **B** As with all organic compounds, C and H are written first in the molecular formula. Adding appropriate subscripts gives the molecular formula $\text{C}_2\text{H}_6\text{O}_2$.
- A** The condensed structural formula shows that trimethylamine contains three CH_3 units, so we have one nitrogen atom, three carbon atoms, and nine hydrogen atoms per molecule. Because trimethylamine contains mostly carbon and hydrogen, it is an organic compound. **B** According to the convention for organic compounds, C and H are written first, giving the molecular formula $\text{C}_3\text{H}_9\text{N}$.

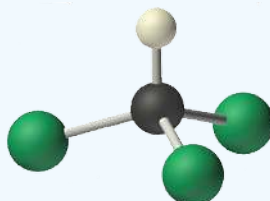


Trimethylamine

? Exercise 1.1.2.2: Molecular Formulas

Write the molecular formula for each molecule.

- Chloroform, which was one of the first anesthetics and was used in many cough syrups until recently, contains one carbon atom, one hydrogen atom, and three chlorine atoms. Its condensed structural formula is CHCl_3 .
- Hydrazine is used as a propellant in the attitude jets of the space shuttle. Its condensed structural formula is H_2NNH_2 .
- Putrescine is a pungent-smelling compound first isolated from extracts of rotting meat. Its condensed structural formula is $\text{H}_2\text{NCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{NH}_2$. This is often written as $\text{H}_2\text{N}(\text{CH}_2)_4\text{NH}_2$ to indicate that there are four CH_2 fragments linked together.



Chloroform

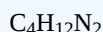
Answer a



Answer b



Answer c



Summary

There are two fundamentally different kinds of chemical bonds (covalent and ionic) that cause substances to have very different properties. The atoms in chemical compounds are held together by attractive electrostatic interactions known as chemical bonds. The molecular formula of a covalent compound gives the types and numbers of atoms present. Compounds that contain predominantly carbon and hydrogen are called organic compounds, whereas compounds that consist primarily of elements other than carbon and hydrogen are inorganic compounds. Diatomic molecules contain two atoms, and polyatomic molecules contain more than two. A structural formula indicates the composition and approximate structure and shape of a molecule. Covalent molecular compounds, in contrast, consist of discrete molecules held together by weak intermolecular forces and can be gases, liquids, or solids at room temperature and pressure.

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1.1.3: Prelude to Organic Chemistry

Scientists of the 18th and early 19th centuries studied compounds obtained from plants and animals and labeled them *organic* because they were isolated from “organized” (living) systems. Compounds isolated from nonliving systems, such as rocks and ores, the atmosphere, and the oceans, were labeled *inorganic*. For many years, scientists thought organic compounds could be made by only living organisms because they possessed a vital force found only in living systems. The vital force theory began to decline in 1828, when the German chemist Friedrich Wöhler synthesized urea from inorganic starting materials. He reacted silver cyanate (AgOCN) and ammonium chloride (NH_4Cl), expecting to get ammonium cyanate (NH_4OCN). What he expected is described by the following equation.



Instead, he found the product to be urea (NH_2CONH_2), a well-known organic material readily isolated from urine. This result led to a series of experiments in which a wide variety of organic compounds were made from inorganic starting materials. The vital force theory gradually went away as chemists learned that they could make many organic compounds in the laboratory.

Today **organic chemistry** is the study of the chemistry of the carbon compounds, and inorganic chemistry is the study of the chemistry of all other elements. It may seem strange that we divide chemistry into two branches—one that considers compounds of only one element and one that covers the 100-plus remaining elements. However, this division seems more reasonable when we consider that of tens of millions of compounds that have been characterized, the overwhelming majority are carbon compounds.

The word *organic* has different meanings. Organic fertilizer, such as cow manure, is organic in the original sense; it is derived from living organisms. Organic foods generally are foods grown without synthetic pesticides or fertilizers. Organic chemistry is the chemistry of compounds of carbon.

Carbon is unique among the other elements in that its atoms can form stable covalent bonds with each other and with atoms of other elements in a multitude of variations. The resulting molecules can contain from one to millions of carbon atoms. We previously surveyed organic chemistry by dividing its compounds into families based on functional groups. We begin with the simplest members of a family and then move on to molecules that are organic in the original sense—that is, they are made by and found in living organisms. These complex molecules (all containing carbon) determine the forms and functions of living systems and are the subject of biochemistry.



Figure 1.1.3.1 All organic compounds contain carbon and most are formed by living things, although they are also formed by geological and artificial processes. (credit left: modification of work by Jon Sullivan; credit left middle: modification of work by Deb Tremper; credit right middle: modification of work by “annszyp”/Wikimedia Commons; credit right: modification of work by George Shuklin)

Organic compounds, like inorganic compounds, obey all the natural laws. Often there is no clear distinction in the chemical or physical properties among organic and inorganic molecules. Nevertheless, it is useful to compare typical members of each class, as in Table 1.1.3.1.

Table 1.1.3.1: General Contrasting Properties and Examples of Organic and Inorganic Compounds

Organic	Hexane	Inorganic	NaCl
low melting points	−95°C	high melting points	801°C
low boiling points	69°C	high boiling points	1,413°C

Organic		Inorganic	
Hexane		NaCl	
low solubility in water; high solubility in nonpolar solvents	insoluble in water; soluble in gasoline	greater solubility in water; low solubility in nonpolar solvents	soluble in water; insoluble in gasoline
flammable	highly flammable	nonflammable	nonflammable
aqueous solutions do not conduct electricity	nonconductive	aqueous solutions conduct electricity	conductive in aqueous solution
exhibit covalent bonding	covalent bonds	exhibit ionic bonding	ionic bonds

Keep in mind, however, that there are exceptions to every category in this table. To further illustrate typical differences among organic and inorganic compounds, Table 1.1.3.1 also lists properties of the inorganic compound sodium chloride (common table salt, NaCl) and the organic compound hexane (C_6H_{14}), a solvent that is used to extract soybean oil from soybeans (among other uses). Many compounds can be classified as organic or inorganic by the presence or absence of certain typical properties, as illustrated in Table 1.1.3.1.

Today, organic compounds are key components of plastics, soaps, perfumes, sweeteners, fabrics, pharmaceuticals, and many other substances that we use every day. The value to us of organic compounds ensures that organic chemistry is an important discipline within the general field of chemistry. In this chapter, we discuss why the element carbon gives rise to a vast number and variety of compounds, how those compounds are classified, and the role of organic compounds in representative biological and industrial settings.

Contributors and Attributions

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- TextMap: The Basics of GOB Chemistry (Ball et al.)

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1.2: Representing Structures

Before we look specifically at several important groups of molecules, we need to understand how chemists symbolically represent chemical structures and how to interpret them. This section focuses on how we represent the organic molecules that make up our body and foods we eat.

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1.2.1: Some Simple Organic Compounds

Learning Objectives

- To be familiar with the classes of basic organic chemistry compounds

Approximately one-third of the compounds produced industrially are organic compounds. All living organisms are composed of organic compounds, as are most foods, medicines, clothing fibers, and plastics. The detection of organic compounds is useful in many fields. In one recently developed application, scientists have devised a new method called “material degradomics” to monitor the degradation of old books and historical documents. As paper ages, it produces a familiar “old book smell” from the release of organic compounds in gaseous form. The composition of the gas depends on the original type of paper used, a book’s binding, and the applied media. By analyzing these organic gases and isolating the individual components, preservationists are better able to determine the condition of an object and those books and documents most in need of immediate protection.

The simplest class of organic compounds is the hydrocarbons, which consist entirely of carbon and hydrogen. Petroleum and natural gas are complex, naturally occurring mixtures of many different hydrocarbons that furnish raw materials for the chemical industry. The four major classes of hydrocarbons are the following: the alkanes, which contain only carbon–hydrogen and carbon–carbon single bonds; the alkenes, which contain at least one carbon–carbon double bond; the alkynes, which contain at least one carbon–carbon triple bond; and the aromatic hydrocarbons, which usually contain rings of six carbon atoms that can be drawn with alternating single and double bonds. Alkanes are also called saturated hydrocarbons, whereas hydrocarbons that contain multiple bonds (alkenes, alkynes, and aromatics) are unsaturated.

Alkanes

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1.2.2: Aliphatic Hydrocarbons

Learning Objectives

- Define and identify alkanes, alkenes, alkynes, and cyclic hydrocarbons.
- List some properties of hydrocarbons.
- Identify and name simple (straight-chain) alkanes given formulas and write formulas for straight-chain alkanes given their names.
- Define structural and geometric isomers.
- Write condensed structural formulas and draw line-angle formulas given complete structural formulas for alkanes, alkenes, alkynes, and cyclic hydrocarbons.

The simplest organic compounds are those composed of only two elements: carbon and hydrogen. These compounds are called **hydrocarbons**. Hydrocarbons themselves are separated into two types: aliphatic hydrocarbons and aromatic hydrocarbons. **Aliphatic hydrocarbons** are hydrocarbons based on chains of C atoms. There are three types of aliphatic hydrocarbons. **Alkanes** are aliphatic hydrocarbons with only single covalent bonds. **Alkenes** are hydrocarbons that contain at least one C–C double bond, and **alkynes** are hydrocarbons that contain a C–C triple bond. Occasionally, we find an aliphatic hydrocarbon with a ring of C atoms; these hydrocarbons are called **cycloalkanes** (or *cycloalkenes* or *cycloalkynes*). Because alkanes have the maximum number of H atoms possible according to the rules of covalent bonds, alkanes are also referred to as **saturated hydrocarbons**.

Note

The word *saturated* has the same meaning for hydrocarbons as it does for the dietary fats and oils: the molecule has no carbon-to-carbon double bonds (C=C).

Alkanes

The simplest alkanes have their C atoms bonded in a straight chain; these are called *normal* alkanes. They are named according to the number of C atoms in the chain. The smallest alkane is methane:

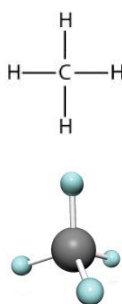
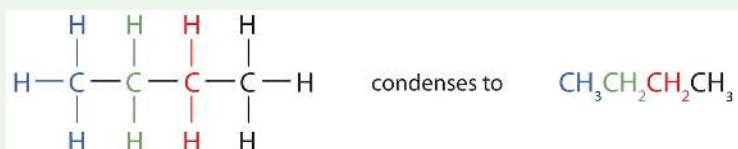


Figure 1.2.2.1. Two dimensional model of methane (top); Three-dimensional representation of methane © Thinkstock. The methane molecule is three dimensional, with the H atoms in the positions of the four corners of a tetrahedron. (bottom)

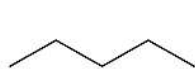
The diagrams representing alkanes are called **structural formulas** because they show the structure of the molecule. As molecules get larger, structural formulas become more and more complex. One way around this is to use a **condensed structural formula**, which lists the formula of each C atom in the backbone of the molecule.

condensed structural formula

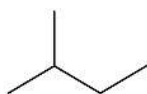
The condensed formulas show hydrogen atoms right next to the carbon atoms to which they are attached, as illustrated for butane:



The ultimate condensed formula is a **line-angle formula (or line drawing)**, in which carbon atoms are implied at the corners and ends of lines, and each carbon atom is understood to be attached to enough hydrogen atoms to give each carbon atom four bonds. For example, we can represent pentane ($\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$) and isopentane [$(\text{CH}_3)_2\text{CHCH}_2\text{CH}_3$] as follows:



Pentane



Isopentane

Table 1.2.2.1 Structural formulas for methane, ethane, and propane

Structural Formula			
Ball and Stick Model			
Space Filling model			
Name	Methane	Ethane	Propane
Condensed Structural Formula	CH_4	CH_3CH_3	$\text{CH}_3\text{CH}_2\text{CH}_3$
Molecular Formula	CH_4	C_2H_6	C_3H_8
Line angle drawing			

✓ Example 1.2.2.1

Provide the molecular formula, the complete structural formula, the condensed structural formula and the line angle formula for a straight chain alkane with 8 carbon atoms.

Solutions

Example 1.2.2.2 writing formulas for a straight chain alkane with eight carbon atoms.

	structural formula	Explanation	Answer
ula	Molecular Formula	The general formula for an alkane is $\text{C}_n\text{H}_{2n+2}$ For an alkane with 8 carbon atoms, $\text{C}_8\text{H}_{(2 \times 8) + 2} = \text{C}_8\text{H}_{18}$.	C_8H_{18} .
ula	Complete Structural Formula	Eight carbons first linked together and all remaining bonds to hydrogen to fulfill the octet rule.	$\text{C}_1\text{-C}_2\text{-C}_3\text{-C}_4\text{-C}_5\text{-C}_6\text{-C}_7\text{-C}_8$

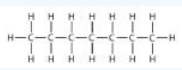
	structural formula	Explanation	Answer
ula	Condensed Structural Formula	The terminal carbon atoms (C_1 and C_8) are bonded to three hydrogen atoms each and the six middle carbon atoms are bonded to two hydrogen atoms each. The six middle carbon atoms are all bonded to two hydrogen atoms so the structural formula can be simplified further.	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2$ $\text{CH}_2\text{CH}_2\text{CH}_3$ $\text{CH}_3(\text{CH}_2)_6\text{CH}_3$
ula	Line Angle Drawing	Eight carbon atoms are implied at the corners and ends of lines, and each carbon atom is understood to be attached to enough hydrogen atoms to give each carbon atom four bonds.	

? Exercise 1.2.2.1

Provide the molecular formula, the complete structural formula, the condensed structural formula, and the line angle formula for a straight chain alkane with 7 carbon atoms.

Answer

molecular formula: C_7H_{16}

complete structural formula: 

condensed structural formula: $\text{CH}_3(\text{CH}_2)_5\text{CH}_3$

line angle drawing: 

Homologous Series

Methane (CH_4), ethane (C_2H_6), and propane (C_3H_8) are the beginning of a series of compounds in which any two members in a sequence differ by one carbon atom and two hydrogen atoms—namely, a CH_2 unit. The first 10 members of this series are given in Table 1.2.2.1.

Table 1.2.2.1 The First 10 Straight-Chain Alkanes

Molecular Formula	Condensed Structural Formula	Name
CH_4	CH_4	methane
C_2H_6	CH_3CH_3	ethane
C_3H_8	$\text{CH}_3\text{CH}_2\text{CH}_3$	propane
C_4H_{10}	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$	butane
C_5H_{12}	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	pentane
C_6H_{14}	$\text{CH}_3(\text{CH}_2)_4\text{CH}_3$	hexane
C_7H_{16}	$\text{CH}_3(\text{CH}_2)_5\text{CH}_3$	heptane
C_8H_{18}	$\text{CH}_3(\text{CH}_2)_6\text{CH}_3$	octane
C_9H_{20}	$\text{CH}_3(\text{CH}_2)_7\text{CH}_3$	nonane
$\text{C}_{10}\text{H}_{22}$	$\text{CH}_3(\text{CH}_2)_8\text{CH}_3$	decane

Note

Parentheses in condensed structural formulas indicate that the enclosed grouping of atoms is attached to the adjacent carbon atom.

Consider the series in Figure 1.2.2.2 The sequence starts with C_3H_8 , and a CH_2 unit is added in each step moving up the series. Any family of compounds in which adjacent members differ from each other by a definite factor (here a CH_2 group) is called a homologous series. The members of such a series, called *homologs*, have properties that vary in a regular and predictable manner. The principle of *homology* gives organization to organic chemistry in much the same way that the periodic table gives organization to inorganic chemistry. Instead of a bewildering array of individual carbon compounds, we can study a few members of a homologous series and from them deduce some of the properties of other compounds in the series.

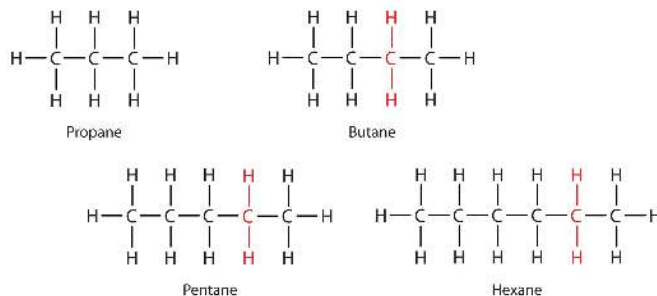


Figure 1.2.2.2 Members of a homologous series.

The principle of homology allows us to write a general formula for alkanes: C_nH_{2n+2} . Using this formula, we can write a molecular formula for any alkane with a given number of carbon atoms. For example, an alkane with eight carbon atoms has the molecular formula $C_8H_{(2 \times 8) + 2} = C_8H_{18}$.

Naming (IUPAC Nomenclature)

A systematic way of naming hydrocarbons and other organic compounds has been devised by the International Union of Pure and Applied Chemistry (IUPAC). These rules, used worldwide, are known as the IUPAC System of Nomenclature. A stem name in Table 1.2.2.1 indicates the number of carbon atoms in the longest continuous chain (LCC). Atoms or groups attached to this carbon chain, called *substituents*, are then named, with their positions indicated by numbers.

Table 1.2.2.2 Stems That Indicate the Number of Carbon Atoms in Organic Molecules

Stem	Number of C Atoms
meth-	1
eth-	2
prop-	3
but-	4
pent-	5
hex-	6
hept-	7
oct-	8
non-	9
dec-	10

Note

A continuous (unbranched) chain of carbon atoms is often called a *straight chain* even though the tetrahedral arrangement about each carbon gives it a zigzag shape. Straight-chain alkanes are sometimes called *normal alkanes*, and their names are given the prefix *n*-. For example, butane is called *n*-butane. We will not use that prefix here because it is not a part of the system established by the International Union of Pure and Applied Chemistry.

✓ Example 1.2.2.2

What is the name of an eight carbon alkane?

Solution

The stem that refers to eight carbon atoms is **oct** plus the suffix **-ane** for an alkane, so the answer is **Octane**.

? Exercise 1.2.2.2

Provide the name for the following compounds:

- seven carbon alkane
- six carbon alkane

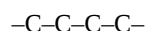
Answer

- heptane
- hexane

Isomerism-Branched Chain Alkanes

One of the interesting aspects of organic chemistry is that it is three-dimensional. A molecule can have a shape in space that may contribute to its properties. Molecules can differ in the way the atoms are arranged - the same combination of atoms can be assembled in more than one way. These compounds are known as **isomers**. Isomers are molecules with the same molecular formulas, but different arrangements of atoms. We will look at some isomer possibilities for alkanes and alkenes.

We can write the structure of butane (C_4H_{10}) by stringing four carbon atoms in a row,



and then adding enough hydrogen atoms to give each carbon atom four bonds:

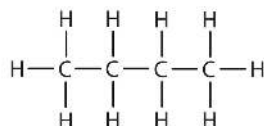


Figure 1.2.2.2 Complete structural formula of butane

The compound butane has this structure, but there is another way to put 4 carbon atoms and 10 hydrogen atoms together. Place 3 of the carbon atoms in a row and then branch the fourth one off the middle carbon atom:

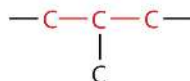
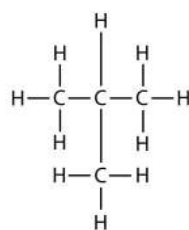


Figure 1.2.2.3 Incomplete structural formula

Now we add enough hydrogen atoms to give each carbon four bonds.



There is a hydrocarbon that corresponds to this structure, which means that two different compounds have the same molecular formula: C_4H_{10} . The two compounds have different properties—for example, one boils at -0.5°C ; the other at -11.7°C . Different compounds having the same molecular formula are called isomers.

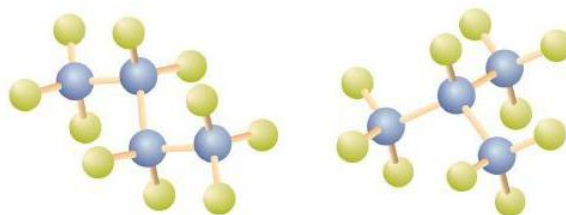
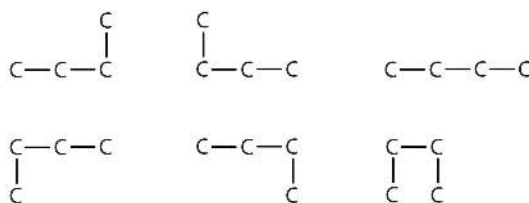


Figure 1.2.2.4 Butane and isobutane. The ball-and-stick models of these two compounds show them to be isomers; both have the molecular formula C_4H_{10} .

Notice that C_4H_{10} is depicted with a bent chain in Figure 1.2.2.4. The four-carbon chain may be bent in various ways because the groups can rotate freely about the C–C bonds. However, this rotation does not change the identity of the compound. It is important to realize that bending a chain does *not* change the identity of the compound; all of the following represent the same compound, butane:



The structure of isobutane shows a continuous chain of three carbon atoms only, with the fourth attached as a branch off the middle carbon atom of the continuous chain, which is different from the structures of butane (compare the two structures in Figure 1.2.2.4).

Unlike C_4H_{10} , the compounds methane (CH_4), ethane (C_2H_6), and propane (C_3H_8) do not exist in isomeric forms because there is only one way to arrange the atoms in each formula so that each carbon atom has four bonds.

Next beyond C_4H_{10} in the homologous series is pentane. Each compound has the same molecular formula: C_5H_{12} . The compound at the far left is pentane because it has all five carbon atoms in a continuous chain. The compound in the middle is isopentane; like isobutane, it has a one CH_3 branch off the second carbon atom of the continuous chain. The compound at the far right, discovered after the other two, was named neopentane (from the Greek *neos*, meaning “new”). Although all three have the same molecular formula, they have different properties, including boiling points: pentane, 36.1°C ; isopentane, 27.7°C ; and neopentane, 9.5°C .

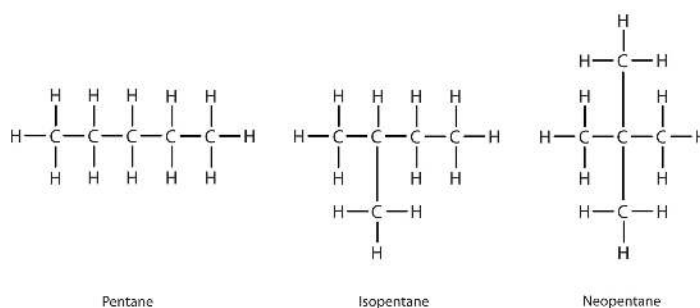


Figure 1.2.2.5 complete structural formulas for pentane isopentane and neopentane

Naming Branched Alkanes

You have already learned the basics of nomenclature-the names of the first 10 normal hydrocarbons. Here, we will add some steps to the procedure so you can name branched hydrocarbons.

First, given the structure of an alkane, identify the longest continuous chain of C atoms. Note that the longest chain may not be drawn in a straight line. The longest chain determines the parent name of the hydrocarbon. For example, in the molecule

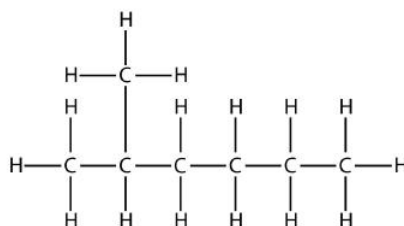


Figure 1.2.2.6 structural formula for hexane

the longest chain of carbons has six C atoms. Therefore, it will be named as a hexane. However, in the molecule

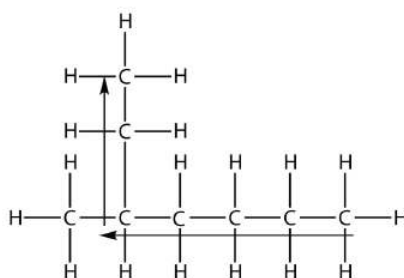


Figure 1.2.2.7 structural formula for heptane

the longest chain of C atoms is not six, but seven, as shown. So this molecule will be named as a heptane.

The next step is to identify the branches, or **substituents**, on the main chain. The names of the substituents, or *alkyl groups*, are derived from the names of the parent hydrocarbons; however, rather than having the ending *-ane*, the substituent name has the ending *-yl*. Table 1.2.2.3 lists the substituent names for the five smallest substituents.

Table 1.2.2.3 Substituent Names.

Substituent Formula	Number of C Atoms	Name of Substituent
CH ₃	1	<i>methyl-</i>
CH ₃ CH ₂	2	<i>ethyl-</i>
CH ₃ CH ₂ CH ₂	3	<i>propyl-</i>
CH ₃ CH ₂ CH ₂ CH ₂	4	<i>butyl-</i>
CH ₃ CH ₂ CH ₂ CH ₂ CH ₂	5	<i>pentyl-</i>
and so forth	and so forth	and so forth

In naming the branched hydrocarbon, the name of the substituent is combined with the parent name of the hydrocarbon without spaces. However, there is likely one more step. The longest chain of the hydrocarbon must be numbered, and the numerical position of the substituent must be included to account for possible isomers. As with double and triple bonds, the main chain is numbered to give the substituent the lowest possible number. For example, in this alkane

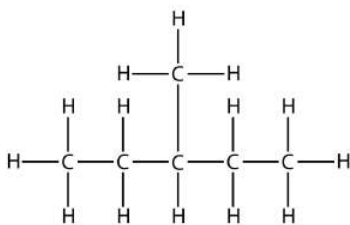


Figure 1.2.2.7 Structural formula for 3-methylpentane

the longest chain is five C atoms long, so it is a pentane. There is a one-carbon substituent on the third C atom, so there is a methyl group at position 3. We indicate the position using the number, which is followed by a hyphen, the substituent name, and the parent hydrocarbon name—in this case, **3-methylpentane**. That name is specific to that particular hydrocarbon and no other molecule. Organic chemistry nomenclature is very specific!

It is common to write the structural formula of a hydrocarbon without the H atoms, for clarity. So we can also represent 3-methylpentane as

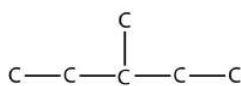
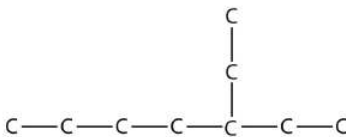


Figure 1.2.2.8 Structural formula for 3-methylpentane without the hydrogen atoms

where it is understood that any unwritten covalent bonds are bonds with H atoms. With this understanding, we recognize that the structural formula for 3-methylpentane refers to a molecule with the formula of C_6H_{14} .

✓ Example 1.2.2.3:

Name this molecule.

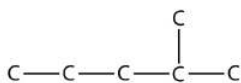


Solution

The longest continuous carbon chain has **seven** C atoms, so this molecule will be named as a **heptane**. There is a **two-carbon substituent** on the main chain, which is an **ethyl group**. To give the substituent the lowest numbering, we number the chain from the *right* side and see that **the substituent is on the third C atom**. So this hydrocarbon is **3-ethylheptane**.

? Exercise 1.2.2.3

Name this molecule.



Answer

2-methylpentane

Branched hydrocarbons may have more than one substituent. If the substituents are different, then give each substituent a number (using the smallest possible numbers) and list the substituents in alphabetical order, with the numbers separated by hyphens and with no spaces in the name. So the molecule

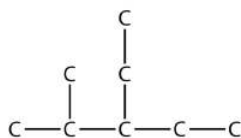


Figure 1.2.2.8 3-ethyl-2-methylpentane

is 3-ethyl-2-methylpentane.

If the substituents are the same, then use the name of the substituent only once, but use more than one number, separated by a comma. Also, put a numerical prefix before the substituent name that indicates the number of substituents of that type. The numerical prefixes are listed in Table 1.2.2.4. The number of the position values must agree with the numerical prefix before the substituent.

Table 1.2.2.4 Numerical Prefixes to Use for Multiple Substituents

Number of Same Substituent	Numerical Prefix
2	<i>di-</i>
3	<i>tri-</i>
4	<i>tetra-</i>
5	<i>penta-</i>
and so forth	and so forth

Consider this molecule:

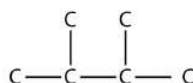
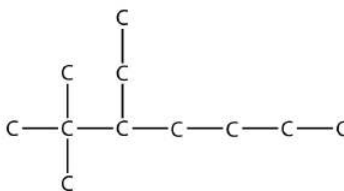


Figure 1.2.2.9 2,3-dimethylbutane

The longest chain has four C atoms, so it is a butane. There are two substituents, each of which consists of a single C atom; they are methyl groups. The methyl groups are on the second and third C atoms in the chain (no matter which end the numbering starts from), so we would name this molecule 2,3-dimethylbutane. Note the comma between the numbers, the hyphen between the numbers and the substituent name, and the presence of the prefix *di-* before the *methyl*. Other molecules—even with larger numbers of substituents—can be named similarly.

✓ Example 1.2.2.4:

Name this molecule.

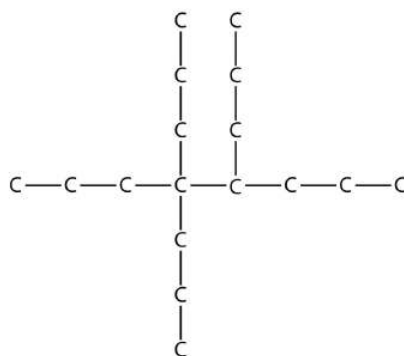


Solution

The longest chain has **seven** C atoms, so we name this molecule as a **heptane**. We find two one-carbon substituents on the second C atom and a **two-carbon substituent** on the third C atom. So this molecule is named **3-ethyl-2,2-dimethylheptane**.

? Exercise 1.2.2.4

Name this molecule.



Answer

4,4,5-tripropyloctane

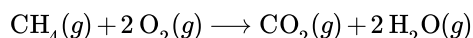
Properties of Alkanes

All alkanes are composed of carbon and hydrogen atoms, and have similar bonds, structures, and formulas; noncyclic alkanes all have a formula of C_nH_{2n+2} . The number of carbon atoms present in an alkane has no limit. Greater numbers of atoms in the molecules will lead to stronger intermolecular attractions (dispersion forces) and correspondingly different physical properties of the molecules. Properties such as melting point and boiling point (Table 1.2.2.5) usually change smoothly and predictably as the number of carbon and hydrogen atoms in the molecules change.

Table 1.2.2.5 Properties of Some Alkanes

Alkane	Molecular Formula	Melting Point (°C)	Boiling Point (°C)	Phase at STP ⁴	Number of Structural Isomers
methane	CH ₄	-182.5	-161.5	gas	1
ethane	C ₂ H ₆	-183.3	-88.6	gas	1
propane	C ₃ H ₈	-187.7	-42.1	gas	1
butane	C ₄ H ₁₀	-138.3	-0.5	gas	2
pentane	C ₅ H ₁₂	-129.7	36.1	liquid	3
hexane	C ₆ H ₁₄	-95.3	68.7	liquid	5
heptane	C ₇ H ₁₆	-90.6	98.4	liquid	9
octane	C ₈ H ₁₈	-56.8	125.7	liquid	18
nonane	C ₉ H ₂₀	-53.6	150.8	liquid	35
decane	C ₁₀ H ₂₂	-29.7	174.0	liquid	75
tetradecane	C ₁₄ H ₃₀	5.9	253.5	solid	1858
octadecane	C ₁₈ H ₃₈	28.2	316.1	solid	60,523

Alkanes are relatively stable molecules, but heat or light will activate reactions that involve the breaking of C-H or C-C single bonds. Combustion is one such reaction:



Alkanes burn in the presence of oxygen, a highly exothermic oxidation-reduction reaction that produces carbon dioxide and water. As a consequence, alkanes are excellent fuels. For example, methane, CH_4 , is the principal component of natural gas. Butane, C_4H_{10} , used in camping stoves and lighters is an alkane. Gasoline is a liquid mixture of continuous- and branched-chain alkanes, each containing from five to nine carbon atoms, plus various additives to improve its performance as a fuel. Kerosene, diesel oil, and fuel oil are primarily mixtures of alkanes with higher molecular masses. The main source of these liquid alkane fuels is crude oil, a complex mixture that is separated by fractional distillation. Fractional distillation takes advantage of differences in the boiling points of the components of the mixture (Figure 1.2.2.10). You may recall that boiling point is a function of intermolecular interactions, which was discussed in the chapter on solutions and colloids.

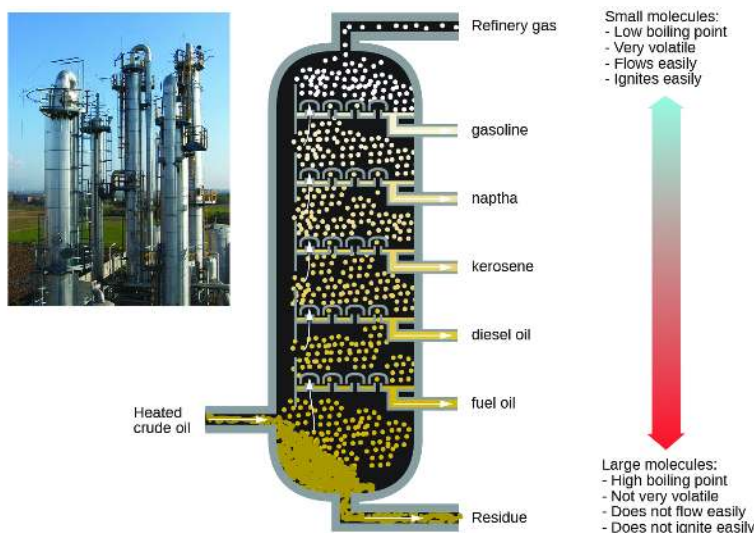


Figure 1.2.2.10 In a column for the fractional distillation of crude oil, oil heated to about 425°C in the furnace vaporizes when it enters the base of the tower. The vapors rise through bubble caps in a series of trays in the tower. As the vapors gradually cool, fractions of higher, then of lower, boiling points condense to liquids and are drawn off. (credit left: modification of work by Luigi Chiesa)

In a substitution reaction, another typical reaction of alkanes, one or more of the alkane's hydrogen atoms is replaced with a different atom or group of atoms. No carbon-carbon bonds are broken in these reactions, and the hybridization of the carbon atoms does not change. For example, the reaction between ethane and molecular chlorine depicted here is a substitution reaction:

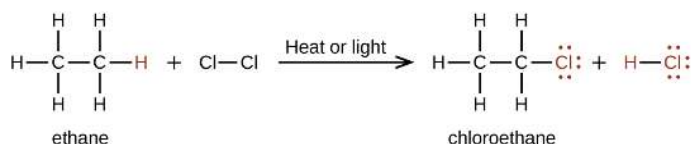


Figure 1.2.2.11 the reaction between ethane and molecular chlorine

The C-Cl portion of the chloroethane molecule is an example of a functional group, the part or moiety of a molecule that imparts a specific chemical reactivity. The types of functional groups present in an organic molecule are major determinants of its chemical properties and are used as a means of classifying organic compounds as detailed in the remaining sections of this chapter.

Cyclic Hydrocarbons

A **cyclic hydrocarbon** is a hydrocarbon in which the carbon chain joins to itself in a ring. A **cycloalkane** is a cyclic hydrocarbon in which all of the carbon-carbon bonds are single bonds. Like other alkanes, cycloalkanes are saturated compounds. Cycloalkanes have the general formula C_nH_{2n} . The simplest cycloalkane shown below is cyclopropane, a three-carbon ring.

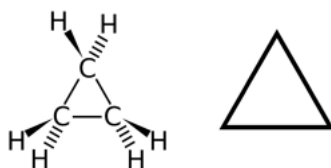


Figure 1.2.2.11 Cyclopropane the simplest cycloalkane.

The structural formulas of cyclic hydrocarbons can be represented in multiple ways, two of which are shown above. Each atom can be shown as in the structure on the left from the figure above. A convenient shorthand is to omit the element symbols and only show the shape, as in the triangle on the right. Carbon atoms are understood to be the vertices of the triangle.

The carbon atoms in cycloalkanes are still sp^3 hybridized, with an ideal bond angle of 109.5° . However, an examination of the cyclopropane structure shows that the triangular structure results in a C—C—C bond angle of 60° . This deviation from the ideal angle is called ring strain and makes cyclopropane a fairly unstable and reactive molecule. Ring strain is decreased for cyclobutane, with a bond angle of 90° , but is still significant. Cyclopentane has a bond angle of about 108° . This minimal ring strain for cyclopentane makes it a more stable compound.

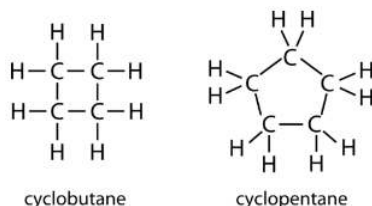


Figure 1.2.2.12 Cyclobutane and Cyclopentane

Cyclohexane is a six-carbon cycloalkane shown below

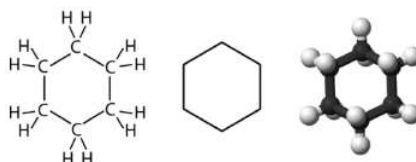


Figure 1.2.2.13 Cyclohexane

All three of the depictions of cyclohexane are somewhat misleading because the molecule is not planar. In order to reduce the ring strain and attain a bond angle of approximately 109.5° , the molecule is puckered. The puckering of the ring means that every other carbon atom is above and below the plane. The figure below shows two possibilities for the puckered cyclohexane molecule. Each of the structures is called a conformation. The conformation on the right is called the boat conformation, while the one on the left is called the chair conformation.



Figure 1.2.2.14 Chair (left) and boat (right) conformations for cyclohexane.

While both conformations reduce the ring strain compared to a planar molecule, the chair is preferred. This is because the chair conformation results in fewer repulsive interactions between the hydrogen atoms. However, interconversion readily occurs between the two conformations.

Larger cycloalkanes also exist, but are less common. Cyclic hydrocarbons may also be unsaturated. A **cycloalkene** is a cyclic hydrocarbon with at least one carbon-carbon double bond. A **cycloalkyne** is a cyclic hydrocarbon with at least one carbon-carbon triple bond. Shown below are the simplified structural formulas for cyclohexene and cyclooctyne.

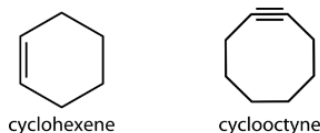


Figure 1.2.2.15 Cyclohexene(left) and cyclooctyne(right)

Unsaturated Hydrocarbons: Alkenes and Alkynes

Alkenes

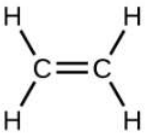
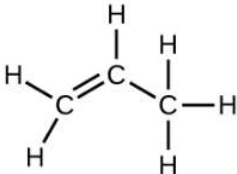
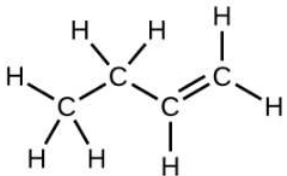
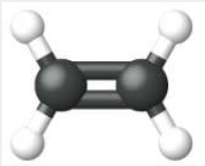
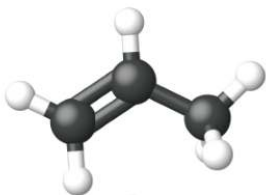
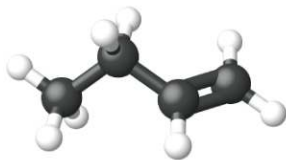
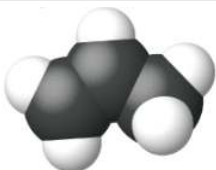
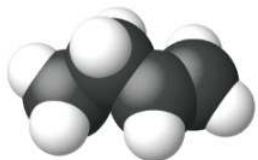
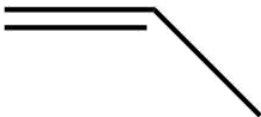
Organic compounds that contain one or more double or triple bonds between carbon atoms are described as unsaturated. Unsaturated hydrocarbons have less than the maximum number of H atoms possible. Unsaturated hydrocarbon molecules that contain one or more double bonds are called alkenes. Carbon atoms linked by a double bond are bound together by two bonds, one σ bond and one π bond. Double and triple bonds give rise to a different geometry around the carbon atom that participates in them, leading to important differences in molecular shape and properties. The differing geometries are responsible for the different properties of unsaturated versus saturated fats.

Note

The word *unsaturated* has the same meaning for hydrocarbons as it does for the dietary fats and oils: the molecule has at least one carbon-to-carbon double ($C=C$) or triple bond ($C\equiv C$).

Ethene, C_2H_4 , is the simplest alkene. Each carbon atom in ethene, commonly called ethylene, has a trigonal planar structure. The second member of the series is propene (propylene) (Figure 1.2.2.10); the butene isomers follow in the series. Four carbon atoms in the chain of butene allows for the formation of isomers based on the position of the double bond, as well as a new form of isomerism.

Structural formulas of Alkenes

Structural Formula			
Ball and Stick Model			
Space Filling model			
Name	ethene	propene	1-butene
Condensed Structural Formula	CH_2CH_2	CH_2CHCH_3	$CH_3CH_2CHCH_2$
Molecular Formula	C_2H_4	C_3H_6	C_4H_8
Line angle drawing			

The name of an alkene is derived from the name of the alkane with the same number of carbon atoms. The presence of the double bond is signified by replacing the suffix *-ane* with the suffix *-ene*. The location of the double bond is identified by naming the smaller of the numbers of the carbon atoms participating in the double bond:

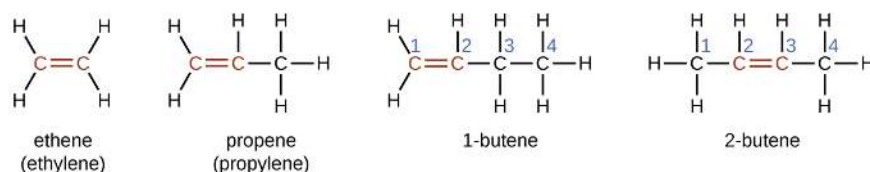


Figure 1.2.2.16 Four structural formulas and names are shown. The first shows two red C atoms connected by a red double bond illustrated with two parallel line segments. H atoms are bonded above and below to the left of the left-most C atom. Two more H atoms are similarly bonded to the right of the C atom on the right. Beneath this structure the name ethene and alternate name ethylene are shown. The second shows three C atoms bonded together with a red double bond between the red first and second C atoms moving left to right across the three-carbon chain. H atoms are bonded above and below to the left of the C atom to the left. A single H is bonded above the middle C atom. Three more H atoms are bonded above, below, and to the right of the third C atom. Beneath this structure the name propene and alternate name propylene is shown. The third shows four C atoms bonded together, numbered one through four moving left to right with a red double bond between the red first and second carbon in the chain. H atoms are bonded above and below to the left of the C atom to the left. A single H is bonded above the second C atom. H atoms are bonded above and below the third C atom. Three more H atoms are bonded above, below, and to the right of the fourth C atom. Beneath this structure the name 1 dash butene is shown. The fourth shows four C atoms bonded together, numbered one through four moving left to right with a red double bond between the red second and third C atoms in the chain. H atoms are bonded above, below, and to the left of the left-most C atom. A single H atom is bonded above the second C atom. A single H atom is bonded above the third C atom. Three more H atoms are bonded above, below, and to the right of the fourth C atom. Beneath this structure the name 2 dash butene is shown.

Alkynes

Hydrocarbon molecules with one or more triple bonds are called alkynes; they make up another series of unsaturated hydrocarbons. Two carbon atoms joined by a triple bond are bound together by one σ bond and two π bonds. The sp -hybridized carbons involved in the triple bond have bond angles of 180° , giving these types of bonds a linear, rod-like shape.

The simplest member of the alkyne series is ethyne, C_2H_2 , commonly called acetylene. The Lewis structure for ethyne, a linear molecule, is:

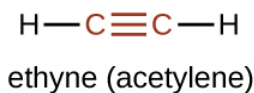


Figure 1.2.2.17 The structural formula and name for ethyne, also known as acetylene, are shown. In red, two C atoms are shown with a triple bond illustrated by three horizontal line segments between them. Shown in black at each end of the structure, a single H atom is bonded.

The IUPAC nomenclature for alkynes is similar to that for alkenes except that the suffix *-yne* is used to indicate a triple bond in the chain. For example, $CH_3CH_2C \equiv CH$ is called 1-butyne.

Naming Alkenes and Alkynes

Alkenes and alkynes are named in a similar fashion. The biggest difference is that when identifying the longest carbon chain, it *must* contain the C-C double or triple bond. Furthermore, when numbering the main chain, the double or triple bond gets the lowest possible number. This means that there may be longer or higher-numbered substituents than may be allowed if the molecule were an alkane. For example, this molecule

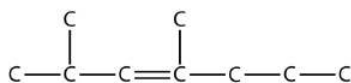
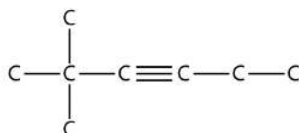


Figure 1.2.2.18 2,4-dimethyl-3-heptene

is 2,4-dimethyl-3-heptene (note the number and the hyphens that indicate the position of the double bond).

✓ Example 1.2.2.5

Name this molecule.

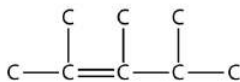


Solution

The longest chain that contains the C–C triple bond has six C atoms, so this is a hexyne molecule. The triple bond starts at the third C atom, so this is a 3-hexyne. Finally, there are two methyl groups on the chain; to give them the lowest possible number, we number the chain from the left side, giving the methyl groups the second position. So the name of this molecule is 2,2-dimethyl-3-hexyne.

? Exercise 1.2.2.5

Name this molecule.



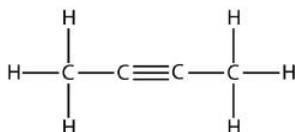
Answer

2,3,4-trimethyl-2-pentene

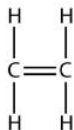
✓ Example 1.2.2.6

Identify the molecule as an alkane, an alkene, or an alkyne.

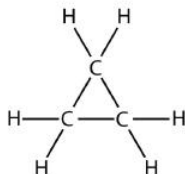
1.



2.



3.



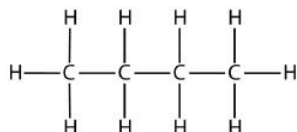
Solution

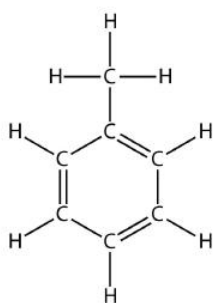
1. The molecule has at least one carbon-to-carbon triple bond ($C\equiv C$) so it is an **alkyne**.
2. The molecule has a one carbon-to-carbon double bond ($C=C$) so it is an **alkene**.
3. The molecule only has carbon-to-carbon single bonds so it is an **alkane**.

? Exercise 1.2.2.6

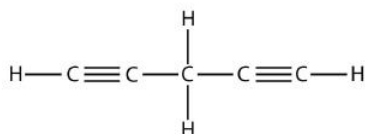
Identify the molecule as an alkane, an alkene, or an alkyne.

1.





2.



3.

Answer

1. alkane, 2. alkene, 3. alkyne

Properties of Alkenes and Alkynes

Ethylene (the common industrial name for ethene) is a basic raw material in the production of polyethylene and other important compounds. Over 135 million tons of ethylene were produced worldwide in 2010 for use in the polymer, petrochemical, and plastic industries. Ethylene is produced industrially in a process called cracking, in which the long hydrocarbon chains in a petroleum mixture are broken into smaller molecules.

Halogens can also react with alkenes and alkynes, but the reaction is different. In these cases, the halogen reacts with the C–C double or triple bond and inserts itself onto each C atom involved in the multiple bonds. This reaction is called an **addition reaction**. One example is

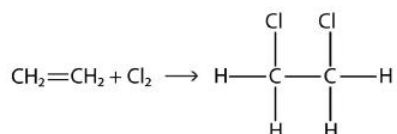
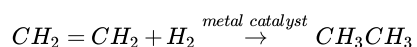
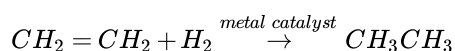


Figure 1.2.2.19



The reaction conditions are usually mild; in many cases, the halogen reacts spontaneously with an alkene or an alkyne.

Hydrogen can also be added across a multiple bond; this reaction is called a **hydrogenation reaction**. In this case, however, the reaction conditions may not be mild; high pressures of H₂ gas may be necessary. A platinum or palladium catalyst is usually employed to get the reaction to proceed at a reasonable pace:



Geometric Isomers (Cis-Trans) Isomers

With a molecule such as 2-butene, a different type of isomerism called geometric isomerism can be observed. **Geometric isomers** are isomers in which the order of atom bonding is the same but the arrangement of atoms in space is different. The double bond in an alkene is not free to rotate because of the nature of the pi bond. Therefore, there are two different ways to construct the 2-butene molecule. The image below shows the two geometric isomers, called *cis*-2-butene and *trans*-2-butene.

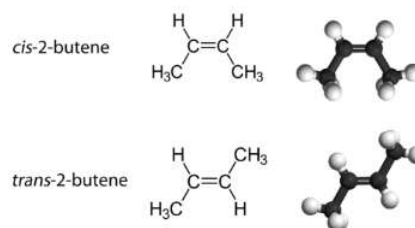


Figure 1.2.2.20\ *cis*-2-butene and *trans*-2-butene.

The ***cis* isomer** has the two single hydrogen atoms on the same side of the molecule, while the ***trans* isomer** has them on opposite sides of the molecule. In both molecules, the bonding order of the atoms is the same. In order for geometric isomers to exist, there must be a rigid structure in the molecule to prevent free rotation around a bond. If the double bond in an alkene was capable of rotating, the two geometric isomers above would not exist. In addition, the two carbon atoms must each have two different groups attached in order for there to be geometric isomers. Propene has no geometric isomers because one of the carbon atoms has two single hydrogens bonded to it.

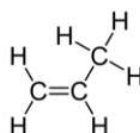


Figure 1.2.2.21\ Propene

Physical and chemical properties of geometric isomers are generally different. While *cis*-2-butene is a polar molecule, *trans*-2-butene is nonpolar. Heat or irradiation with light can be used to bring about the conversion of one geometric isomer to another. The input of energy must be large enough to break the pi bond between the two carbon atoms, which is weaker than the sigma bond. At that point, the now single bond is free to rotate and the isomers can interconvert.

As with alkenes, alkynes display structural isomerism beginning with 1-butyne and 2-butyne. However, there are no geometric isomers with alkynes because there is only one other group bonded to the carbon atoms that are involved in the triple bond.

Summary

- Simple alkanes exist as a homologous series, in which adjacent members differ by a CH₂ unit.
- Condensed chemical formulas show the hydrogen atoms (or other atoms or groups) right next to the carbon atoms to which they are attached.
- Line-angle formulas imply a carbon atom at the corners and ends of lines. Each carbon atom is understood to be attached to enough hydrogen atoms to give each carbon atom four bonds.
- Alkanes have both common names and systematic names, specified by IUPAC.
- Names and structures of typical cyclic hydrocarbons are given.
- Structural and geometric isomers are defined.
- Examples of alkane and alkene isomers are given.

Contributors and Attributions

- OpenSTAX
- TextMap: Beginning Chemistry (Ball et al.)
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1.2.3: The Functional Group

Learning Objectives

- Define *functional group*.
- Identify the functional group(s) present in organic compounds.

With over twenty million known organic compounds in existence, it would be very challenging to memorize chemical reactions for each one. Fortunately, molecules with similar functional groups tend to undergo similar reactions. A **functional group** is defined as an atom or group of atoms within a molecule that has similar chemical properties whenever it appears in various compounds. Even if other parts of the molecule are quite different, certain functional groups tend to react in certain ways.

We've already looked at alkanes, but they are generally unreactive. We primarily use alkanes as a source of energy when they are combusted. While the majority of functional groups involve atoms other than carbon and hydrogen, we will also look at some that include only carbon and hydrogen. Some of the most common functional groups are presented in the following sections.

Organic molecules vary greatly in size and when focusing on functional groups, we want to direct our attention to the atoms involved in the functional group. As a result, the abbreviation **R** is used in some examples. The letter **R** is used in molecular structures to represent the "**R**est of the molecule". It consists of a group of carbon and hydrogen atoms of any size. It is used as an abbreviation since a group of carbon and hydrogen atoms does not affect the functionality of the compound. In some molecules, you will see **R**, **R'**, or **R''** which indicates that the R groups in the molecule can be different from one another. For example, R might be $-\text{CH}_2\text{CH}_3$ while R' is $-\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$.

The structure of capsaicin, the compound responsible for the heat in peppers, incorporates several functional groups, labeled in the figure below and explained throughout this section.

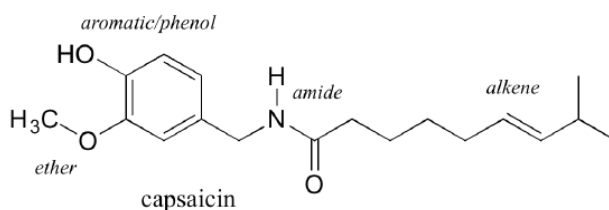


Figure 1.2.3.1 The structure of capsaicin

The table below summarizes the structures that will be discussed in this chapter:

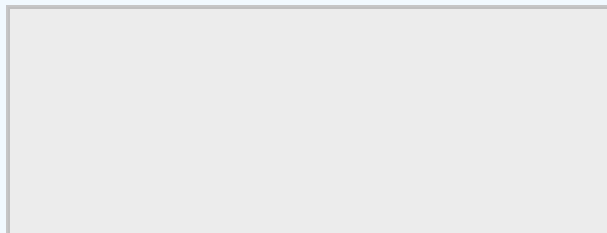
Table 1.2.3.1 Selected Organic Functional Groups

Compound Name	Structure of Compound and Functional Group (red)	Example	
		Formula	Name
alkene	$\text{C}=\text{C}$	C_2H_4	 ethene
alkyne	$\text{C}\equiv\text{C}$	C_2H_2	 ethyne
alcohol	$\text{R}-\ddot{\text{O}}-\text{H}$	$\text{CH}_3\text{CH}_2\text{OH}$	 ethanol
ether	$\text{R}-\ddot{\text{O}}-\text{R}'$	$(\text{C}_2\text{H}_5)_2\text{O}$	 diethyl ether
aldehyde	$\begin{array}{c} \text{:O:} \\ \\ \text{R}-\text{C}-\text{H} \end{array}$	CH_3CHO	 ethanal
ketone	$\begin{array}{c} \text{:O:} \\ \\ \text{R}-\text{C}-\text{R}' \end{array}$	$\text{CH}_3\text{COCH}_2\text{CH}_3$	 methyl ethyl ketone
carboxylic acid	$\begin{array}{c} \text{:O:} \\ \\ \text{R}-\text{C}-\ddot{\text{O}}-\text{H} \end{array}$	CH_3COOH	 acetic acid
ester	$\begin{array}{c} \text{:O:} \\ \\ \text{R}-\text{C}-\ddot{\text{O}}-\text{R}' \end{array}$	$\text{CH}_3\text{CO}_2\text{CH}_2\text{CH}_3$	 ethyl acetate
amine	$\begin{array}{ccc} \text{R}-\ddot{\text{N}}-\text{H} & \text{R}-\ddot{\text{N}}-\text{H} & \text{R}-\ddot{\text{N}}-\text{R}'' \\ & & \\ \text{H} & \text{R}' & \text{R}' \end{array}$	$\text{C}_2\text{H}_5\text{NH}_2$	 ethylamine
amide	$\begin{array}{c} \text{:O:} \\ \\ \text{R}-\text{C}-\ddot{\text{N}}-\text{R}' \\ \\ \text{H} \end{array}$	CH_3CONH_2	 acetamide

Figure 1.2.3.1

✓ Example 1.2.3.1

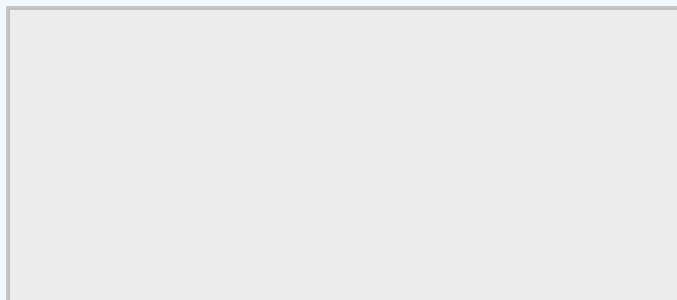
Identify the common functional groups for ATP.



Example 1.2.3.1

Solution

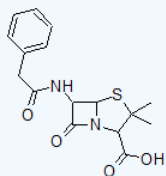
The common functional groups for ATP are **hydroxyl**, **ether** and **amine**. The other functional groups are covered in higher organic chemistry courses.



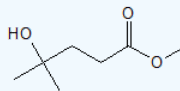
Example 1.2.3.1 ATP

? Exercise 1.2.3.1

Identify the functional groups (other than alkanes) in the following organic compounds. State whether alcohols and amines are primary, secondary, or tertiary.



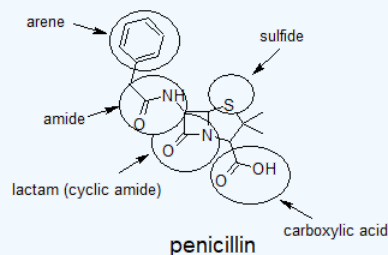
penicillin



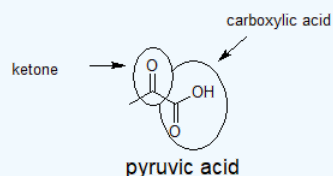
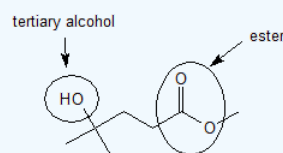
pyruvic acid



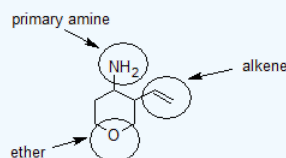
Answer



penicillin



pyruvic acid



Summary

- Functional groups consist of a single atom (such as Cl) or a group of atoms (such as CO₂H). It can determine the chemical reactivity of a molecule under a given set of conditions
- The major families of organic compounds are characterized by their functional groups.

Contributors and Attributions

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1.3: Carbohydrates, Fats and Proteins

The food we eat has three main types of macro-nutrients: carbohydrates (sugars), fats (lipids) and proteins (polymers of amino acids). In this section we will look at the structures and properties of each of these major classes of chemicals.

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1.3.1: Energy and the Living Cell

Learning Objective

- Know the similarities and differences between plant and animal cells.
- Know the functions of the major parts of plant and animal cells.

Biochemistry, sometimes called **biological chemistry**, is the study of chemical processes within and relating to living organisms. Biochemical processes give rise to the complexity of life. Biochemistry focuses on understanding how biological molecules give rise to the processes that occur within living cells and between cells, which in turn relates greatly to the study and understanding of tissues, organs, and organism structure and function. Much of biochemistry deals with the structures, functions and interactions of biological macromolecules, such as proteins, nucleic acids, carbohydrates and lipids, which provide the structure of cells and perform many of the functions associated with life. The mechanisms by which cells harness energy from their environment via chemical reactions are known as metabolism. The findings of biochemistry are applied primarily in medicine, nutrition, and agriculture. In medicine, biochemists investigate the causes and cures of diseases. In nutrition, they study how to maintain health wellness and study the effects of nutritional deficiencies. In agriculture, biochemists investigate soil and fertilizers, and try to discover ways to improve crop cultivation, crop storage and pest control.

The major parts of plant and animal cells (Figure 1.3.1.1) include the plasma membrane, nucleus, ribosomes, and mitochondria.

The plasma membrane is made up of a phospholipid bilayer with embedded proteins that separates the internal contents of the cell from its surrounding environment. A phospholipid is a lipid molecule composed of two fatty acid chains, a glycerol backbone, and a phosphate group. The plasma membrane regulates the passage of some substances, such as organic molecules, ions, and water, preventing the passage of some to maintain internal conditions, while actively bringing in or removing others. Other compounds move passively across the membrane.

Nucleus

Typically, the **nucleus** is the most prominent organelle in a cell. The nucleus (plural = nuclei) houses the cell's DNA in the form of chromatin and directs the synthesis of ribosomes and proteins.

Ribosomes

Ribosomes are the cellular structures responsible for protein synthesis. When viewed through an electron microscope, free ribosomes appear as either clusters or single tiny dots floating freely in the cytoplasm. Ribosomes may be attached to either the cytoplasmic side of the plasma membrane or the cytoplasmic side of the endoplasmic reticulum. Electron microscopy has shown that ribosomes consist of large and small subunits. Ribosomes are enzyme complexes that are responsible for protein synthesis.

Because protein synthesis is essential for all cells, ribosomes are found in practically every cell, although they are smaller in prokaryotic cells. They are particularly abundant in immature red blood cells for the synthesis of hemoglobin, which functions in the transport of oxygen throughout the body.

Mitochondria

Mitochondria (singular = mitochondrion) are often called the “powerhouses” or “energy factories” of a cell because they are responsible for making adenosine triphosphate (ATP), the cell's main energy-carrying molecule. The formation of ATP from the breakdown of glucose is known as cellular respiration. In keeping with our theme of form following function, it is important to point out that muscle cells have a very high concentration of mitochondria because muscle cells need a lot of energy to contract.

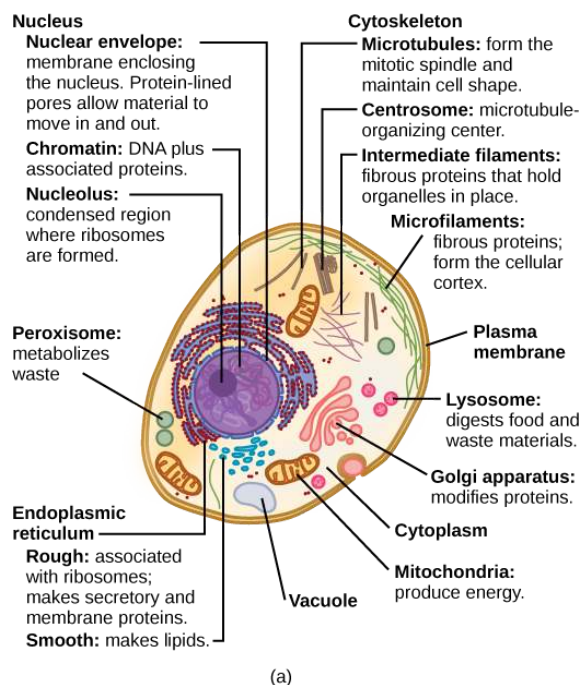


Figure_03_03_01b_new.png?revision=1&size=bestfit&width=519&height=476" style="width: 490.994px; height: 450px;"/>

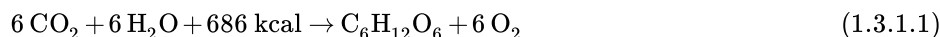
Figure 1.3.1.1: This figure shows (a) a typical animal cell and (b) a typical plant cell.

Animal Cells versus Plant Cells

Despite their fundamental similarities, there are some striking differences between animal and plant cells. Animal cells have centrioles, centrosomes (discussed under the cytoskeleton), and lysosomes, whereas plant cells do not. Plant cells have a cell wall (made of cellulose), chloroplasts, plasmodesmata, and plastids used for storage, and a large central vacuole, whereas animal cells do not.

Energy in Biological Systems

Green plants are capable of synthesizing glucose ($C_6H_{12}O_6$) from carbon dioxide (CO_2) and water (H_2O) by using solar energy in the process known as photosynthesis:



(The 686 kcal come from solar energy.) Chloroplasts function in photosynthesis and can be found in cells of plants and algae. The chloroplasts contain a green pigment called chlorophyll, which captures the energy of sunlight for photosynthesis. Plants can use the glucose for energy or convert it to larger carbohydrates, such as starch or cellulose. Starch provides energy for later use, perhaps as nourishment for a plant's seeds, while cellulose is the structural material of plants. We can gather and eat the parts of a plant that store energy—seeds, roots, tubers, and fruits—and use some of that energy ourselves. Carbohydrates are also needed for the synthesis of nucleic acids and many proteins and lipids. This is the major difference between plants and animals: Plants are able to make their own food, like glucose, whereas animals must rely on other organisms for their organic compounds or food source.

Summary

The major parts of plant and animal cells (Figure 1.3.1.1) include the plasma membrane, nucleus, ribosomes, and mitochondria.

Animal cells have centrioles, centrosomes (discussed under the cytoskeleton), and lysosomes, whereas plant cells do not.

Plant cells have a cell wall (made of cellulose), chloroplasts, plasmodesmata, and plastids used for storage, and a large central vacuole, whereas animal cells do not.

Green plants are capable of synthesizing glucose ($C_6H_{12}O_6$) from carbon dioxide (CO_2) and water (H_2O) by using solar energy in the process known as photosynthesis.

Contributors and Attributions

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1.3.2: Carbohydrates- A Storehouse of Energy

Learning Objective

- Know the difference between starch, cellulose and glycogen.
- List the key steps in carbohydrate digestion.

All carbohydrates consist of carbon, hydrogen, and oxygen atoms and are polyhydroxy aldehydes or ketones or are compounds that can be broken down to form such compounds. Examples of carbohydrates include starch, fiber, the sweet-tasting compounds called sugars, and structural materials such as cellulose. Different carbohydrates that will be discussed below include the simple sugars, oligosaccharides and polysaccharides (Figure 1.3.2.1).

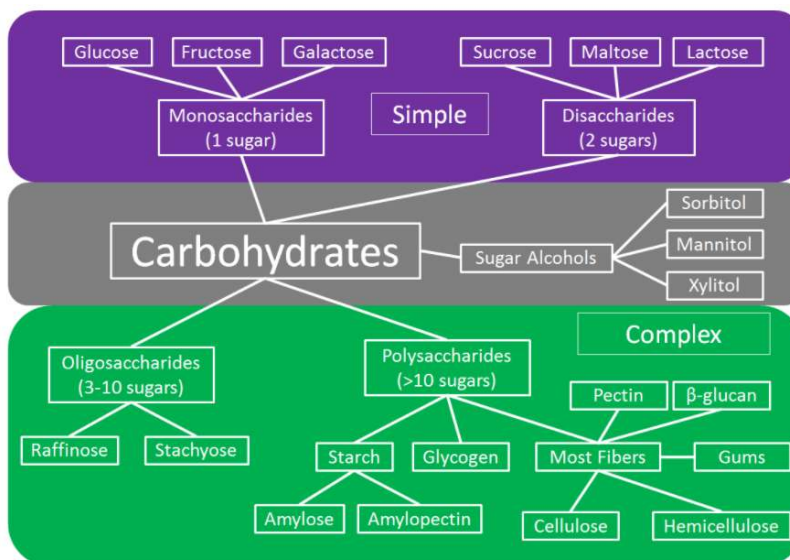
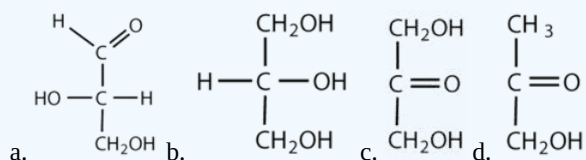


Figure 1.3.2.1 Overview of carbohydrates

✓ Example 1.3.2.1

Which compounds would be classified as carbohydrates?

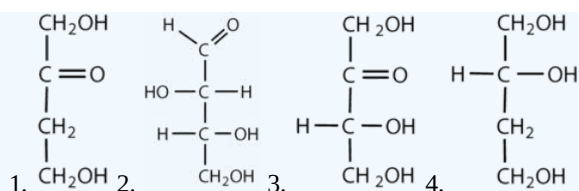


Solution

- This is a carbohydrate because the molecule contains an aldehyde functional group with OH groups on the other two carbon atoms.
- This is not a carbohydrate because the molecule does not contain an aldehyde or a ketone functional group.
- This is a carbohydrate because the molecule contains a ketone functional group with OH groups on the other two carbon atoms.
- This is not a carbohydrate; although it has a ketone functional group, one of the other carbons atoms does not have an OH group attached.

? Exercise 1.3.2.1

Which compounds would be classified as carbohydrates?



Some Simple Sugars

The naturally occurring **monosaccharides** contain three to seven carbon atoms per molecule (one sugar unit) . Monosaccharides (or simple sugars) of specific sizes may be indicated by names composed of a stem denoting the number of carbon atoms and the suffix *-ose*. For example, the terms *triose*, *tetrose*, *pentose*, and *hexose* signify monosaccharides with, respectively, three, four, five, and six carbon atoms. Monosaccharides are also classified as aldoses or ketoses. Those monosaccharides that contain an aldehyde functional group are called aldoses; those containing a ketone functional group on the second carbon atom are ketoses. Combining these classification systems gives general names that indicate both the type of carbonyl group *and* the number of carbon atoms in a molecule. Thus, monosaccharides are described as aldotetroses, aldopentoses, ketopentoses, ketoheptoses, and so forth.

Although a variety of monosaccharides are found in living organisms, three hexoses are particularly abundant: D-glucose, D-galactose, and D-fructose (Figure 1.3.2.2). Glucose and galactose are both aldohexoses, while fructose is a ketohexose.

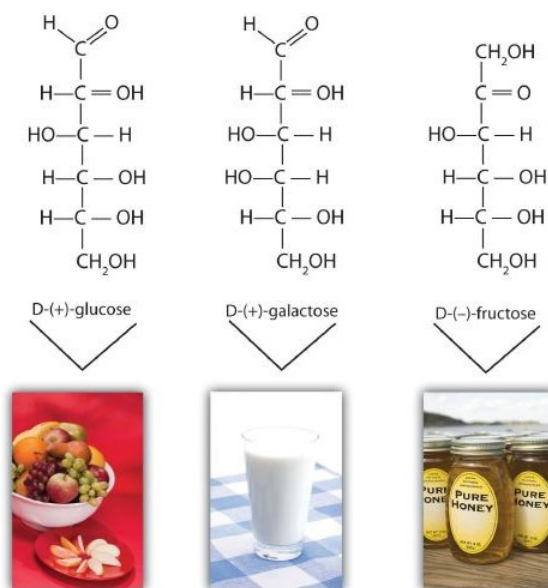


Figure 1.3.2.2: Structures of Three Important Hexoses. Each hexose is pictured with a food source in which it is commonly found.
Source: Photos © Thinkstock.

In aqueous solution, the predominant forms are not the straight-chain structure shown above. Rather, they adopt a cyclic structure. The representative ring structures of glucose, fructose, and galactose are shown in Figure 1.3.2.3 Notice that all are 6-carbon sugars (hexoses). However, fructose has a five member ring, while glucose and galactose have 6 member rings. Also notice that the only structural difference between glucose and galactose is the position of the alcohol (OH) group that is shown in red.

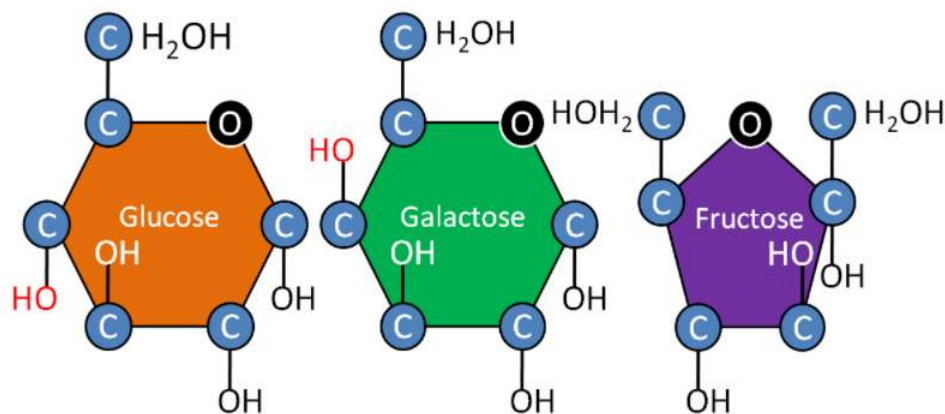


Figure 1.3.2.3 The ring structures of glucose, galactose, and fructose.

A **disaccharide** contains two monosaccharides joined together. Examples include and . They are composed of two monosaccharide units bound together by a bond known as a formed via a , resulting in the loss of a atom from one monosaccharide and a from the other. The of unmodified disaccharides is $C_{12}H_{22}O_{11}$. Although there are numerous kinds of disaccharides, a handful of disaccharides are particularly notable.

Sucrose, which may be obtained by condensing a molecule of α -glucose with one of the cyclic forms of fructose called β -fructose. The structure of sucrose is shown in Figure 1.3.2.4

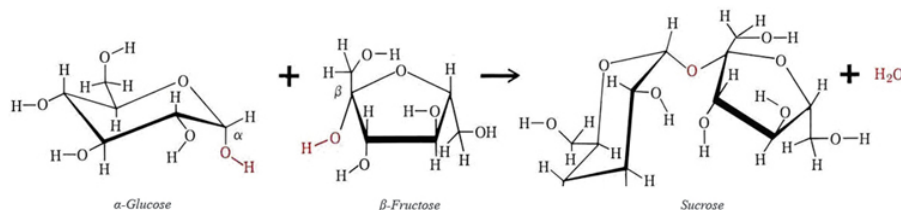


Figure 1.3.2.4 The formation of sucrose from glucose and fructose.

Other, less familiar, examples of disaccharides are lactose, which occurs in milk, and maltose, which are shown in Figure 1.3.2.5 In order to digest a disaccharide like sucrose or lactose, the human body must have an enzyme which can catalyze hydrolysis of the linkage between the two monosaccharide units. Many Asians, Africans, and American Indians are incapable of synthesizing lactase, the enzyme that speeds hydrolysis of lactose. If such persons drink milk, the undigested lactose makes them sick.

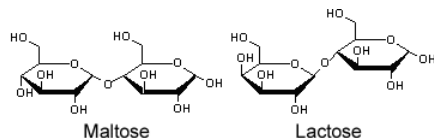


Figure 1.3.2.5 Two other common disaccharides, maltose and lactose.

The polysaccharides are the most abundant carbohydrates in nature and serve a variety of functions, such as energy storage or as components of plant cell walls. Polysaccharides are very large polymers composed of tens to thousands of monosaccharides joined together by glycosidic linkages. The three most abundant polysaccharides are starch, glycogen, and cellulose. These three are referred to as *homopolymers* because each yields only one type of monosaccharide (glucose) after complete hydrolysis. *Heteropolymers* may contain sugar acids, amino sugars, or noncarbohydrate substances in addition to monosaccharides. Heteropolymers are common in nature (gums, pectins, and other substances) but will not be discussed further in this textbook. The polysaccharides are nonreducing carbohydrates, are not sweet tasting, and do not undergo mutarotation.

Starch

Starch is the most important source of carbohydrates in the human diet and accounts for more than 50% of our carbohydrate intake. It occurs in plants in the form of granules, and these are particularly abundant in seeds (especially the cereal grains) and tubers, where they serve as a storage form of carbohydrates. The breakdown of starch to glucose nourishes the plant during periods of reduced photosynthetic activity. We often think of potatoes as a “starchy” food, yet other plants contain a much greater percentage of starch (potatoes 15%, wheat 55%, corn 65%, and rice 75%). Commercial starch is a white powder.

Starch is a mixture of two polymers: amylose and amylopectin. Natural starches consist of about 10%–30% amylose and 70%–90% amylopectin. Amylose is a linear polysaccharide composed entirely of D-glucose units joined by the α -1,4-glycosidic linkages we saw in maltose (part (a) of Figure 1.3.2.6). Experimental evidence indicates that amylose is not a straight chain of glucose units but instead is coiled like a spring, with six glucose monomers per turn (part (b) of Figure 1.3.2.6). When coiled in this fashion, amylose has just enough room in its core to accommodate an iodine molecule. The characteristic blue-violet color that appears when starch is treated with iodine is due to the formation of the amylose-iodine complex. This color test is sensitive enough to detect even minute amounts of starch in solution.

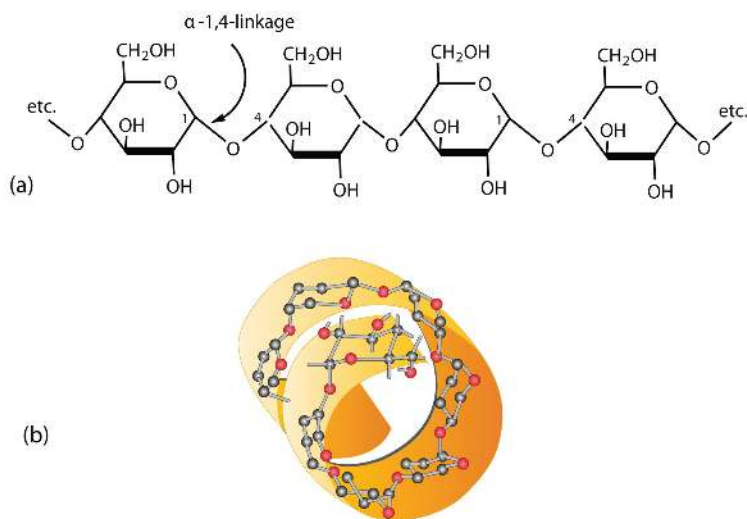


Figure 1.3.2.6 Amylose. (a) Amylose is a linear chain of α -D-glucose units joined together by α -1,4-glycosidic bonds. (b) Because of hydrogen bonding, amylose acquires a spiral structure that contains six glucose units per turn.

Amylopectin is a branched-chain polysaccharide composed of glucose units linked primarily by α -1,4-glycosidic bonds but with occasional α -1,6-glycosidic bonds, which are responsible for the branching. A molecule of amylopectin may contain many thousands of glucose units with branch points occurring about every 25–30 units (Figure 1.3.2.7). The helical structure of amylopectin is disrupted by the branching of the chain, so instead of the deep blue-violet color amylose gives with iodine, amylopectin produces a less intense reddish brown.

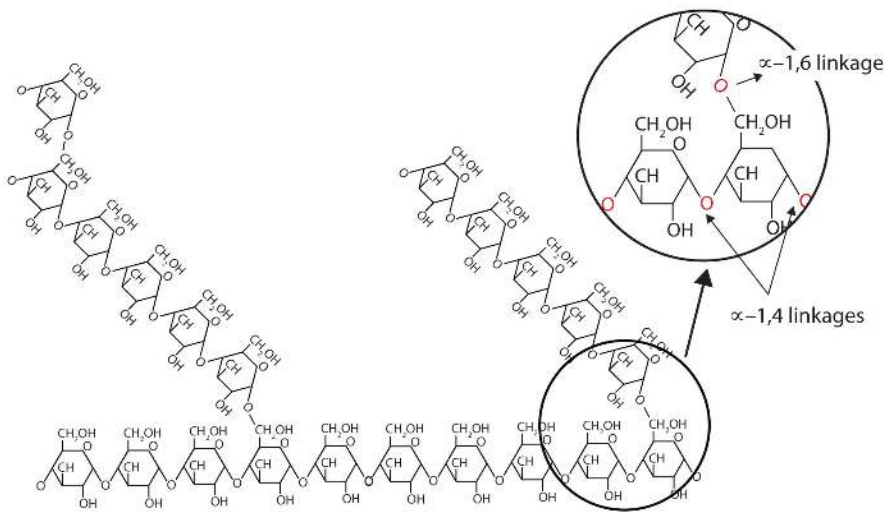
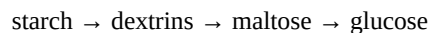


Figure 1.3.2.7 Representation of the Branching in Amylopectin and Glycogen. Both amylopectin and glycogen contain branch points that are linked through α -1,6-linkages. These branch points occur more often in glycogen.

Dextrins are glucose polysaccharides of intermediate size. The shine and stiffness imparted to clothing by starch are due to the presence of dextrins formed when clothing is ironed. Because of their characteristic stickiness with wetting, dextrins are used as adhesives on stamps, envelopes, and labels; as binders to hold pills and tablets together; and as pastes. Dextrins are more easily digested than starch and are therefore used extensively in the commercial preparation of infant foods.

The complete hydrolysis of starch yields, in successive stages, glucose:



In the human body, several enzymes known collectively as amylases degrade starch sequentially into usable glucose units.

Glycogen

Glycogen is the energy reserve carbohydrate of animals. Practically all mammalian cells contain some stored carbohydrates in the form of glycogen, but it is especially abundant in the liver (4%–8% by weight of tissue) and in skeletal muscle cells (0.5%–1.0%). Like starch in plants, glycogen is found as granules in liver and muscle cells. When fasting, animals draw on these glycogen reserves during the first day without food to obtain the glucose needed to maintain metabolic balance.

Glycogen is structurally quite similar to amylopectin, although glycogen is more highly branched (8–12 glucose units between branches) and the branches are shorter. When treated with iodine, glycogen gives a reddish brown color. Glycogen can be broken down into its D-glucose subunits by acid hydrolysis or by the same enzymes that catalyze the breakdown of starch. In animals, the enzyme phosphorylase catalyzes the breakdown of glycogen to phosphate esters of glucose.

About 70% of the total glycogen in the body is stored in muscle cells. Although the percentage of glycogen (by weight) is higher in the liver, the much greater mass of skeletal muscle stores a greater total amount of glycogen.

Cellulose

Cellulose, a fibrous carbohydrate found in all plants, is the structural component of plant cell walls. Because the earth is covered with vegetation, cellulose is the most abundant of all carbohydrates, accounting for over 50% of all the carbon found in the vegetable kingdom. Cotton fibrils and filter paper are almost entirely cellulose (about 95%), wood is about 50% cellulose, and the dry weight of leaves is about 10%–20% cellulose. The largest use of cellulose is in the manufacture of paper and paper products. Although the use of noncellulose synthetic fibers is increasing, rayon (made from cellulose) and cotton still account for over 70% of textile production.

Like amylose, cellulose is a linear polymer of glucose. It differs, however, in that the glucose units are joined by β -1,4-glycosidic linkages, producing a more extended structure than amylose (part (a) of Figure 1.3.2.8). This extreme linearity allows a great deal of hydrogen bonding between OH groups on adjacent chains, causing them to pack closely into fibers (part (b) of Figure 1.3.2.8). As a result, cellulose exhibits little interaction with water or any other solvent. Cotton and wood, for example, are completely insoluble in water and have considerable mechanical strength. Because cellulose does not have a helical structure, it does not bind to iodine to form a colored product.

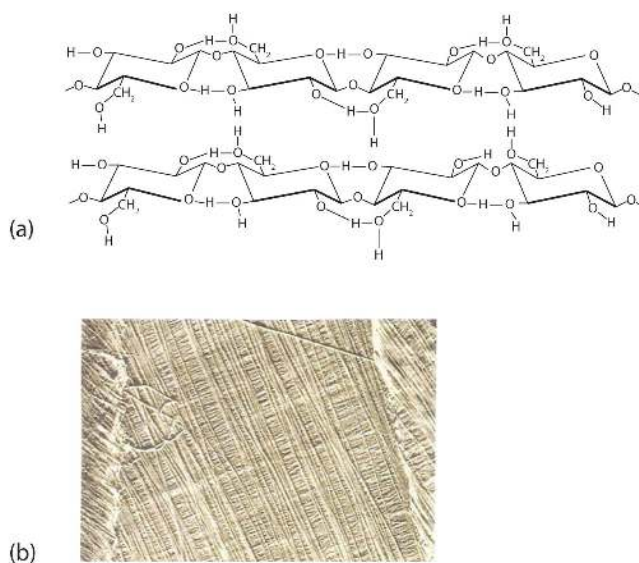


Figure 1.3.2.8 Cellulose. (a) There is extensive hydrogen bonding in the structure of cellulose. (b) In this electron micrograph of the cell wall of an alga, the wall consists of successive layers of cellulose fibers in parallel arrangement.

Cellulose yields D-glucose after complete acid hydrolysis, yet humans are unable to metabolize cellulose as a source of glucose. Our digestive juices lack enzymes that can hydrolyze the β -glycosidic linkages found in cellulose, so although we can eat potatoes, we cannot eat grass. However, certain microorganisms can digest cellulose because they make the enzyme cellulase, which catalyzes the hydrolysis of cellulose. The presence of these microorganisms in the digestive tracts of herbivorous animals (such as cows, horses, and sheep) allows these animals to degrade the cellulose from plant material into glucose for energy. Termites also contain cellulase-secreting microorganisms and thus can subsist on a wood diet. This example once again demonstrates the extreme stereospecificity of biochemical processes.

Summary

- Starch is a storage form of energy in plants. It contains two polymers composed of glucose units: amylose (linear) and amylopectin (branched).
- Glycogen is a storage form of energy in animals. It is a branched polymer composed of glucose units. It is more highly branched than amylopectin.
- Cellulose is a structural polymer of glucose units found in plants. It is a linear polymer with the glucose units linked through β -1,4-glycosidic bonds.

Sources

Wikipedia

Contributors and Attributions

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1.3.3: Fats and Other Lipids

Learning Objectives

- Recognize the structures of common fatty acids.
- Describe the structure of fats and oils and classify them as saturated, monounsaturated, or polyunsaturated.

Fats and oils, found in many of the foods we eat, belong to a class of biomolecules known as lipids. Gram for gram, they pack more than twice the caloric content of carbohydrates: the oxidation of fats and oils supplies about 9 kcal of energy for every gram oxidized, whereas the oxidation of carbohydrates supplies only 4 kcal/g. Although the high caloric content of fats may be bad news for the dieter, it says something about the efficiency of nature's designs. Our bodies use carbohydrates, primarily in the form of glucose, for our *immediate* energy needs. Our capacity for storing carbohydrates for later use is limited to tucking away a bit of glycogen in the liver or in muscle tissue. We store our *reserve* energy in lipid form, which requires far less space than the same amount of energy stored in carbohydrate form. Lipids have other biological functions besides energy storage. They are a major component of the membranes of the 10 trillion cells in our bodies. They serve as protective padding and insulation for vital organs. Furthermore, without lipids in our diets, we would be deficient in the fat-soluble vitamins A, D, E, and K.

Lipids are not defined by the presence of specific functional groups, as carbohydrates are, but by a physical property—solubility. Compounds isolated from body tissues are classified as lipids if they are more soluble in organic solvents, such as dichloromethane, than in water. By this criterion, the lipid category includes not only fats and oils, which are esters of the trihydroxy alcohol glycerol and fatty acids, but also compounds that incorporate functional groups derived from phosphoric acid, carbohydrates, or amino alcohols, as well as steroid compounds such as cholesterol (Figure 1.3.3.1 presents one scheme for classifying the various kinds of lipids). We will discuss the various kinds of lipids by considering one subclass at a time and pointing out structural similarities and differences as we go.

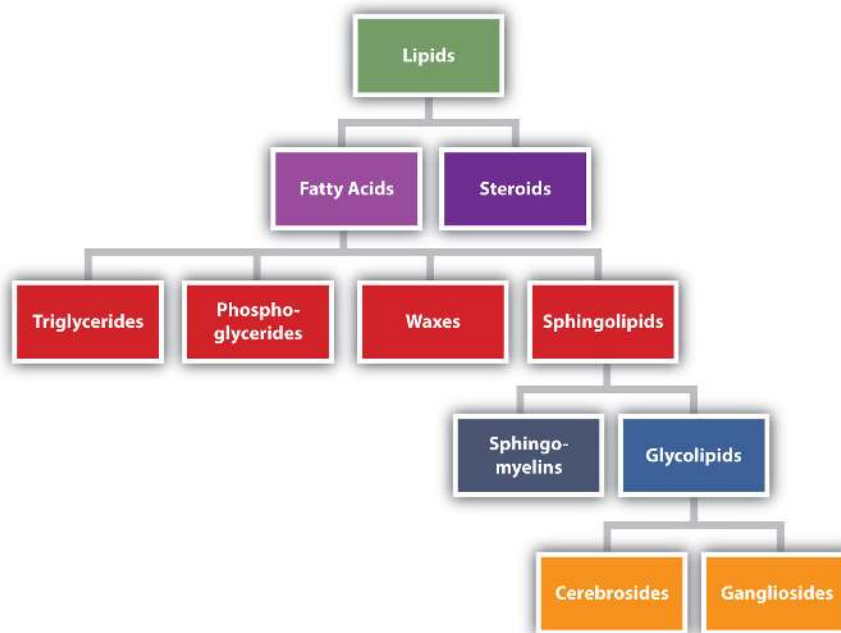


Figure 1.3.3.1 Lipid organization based on structural relationships

Fatty Acids

Fatty acids are carboxylic acids that are structural components of fats, oils, and all other categories of lipids, except steroids. More than 70 have been identified in nature. They usually contain an even number of carbon atoms (typically 12–20), are generally unbranched, and can be classified by the presence and number of carbon-to-carbon double bonds. Thus, saturated fatty acids contain no carbon-to-carbon double bonds, monounsaturated fatty acids contain one carbon-to-carbon double bond, and polyunsaturated fatty acids contain two or more carbon-to-carbon double bonds.

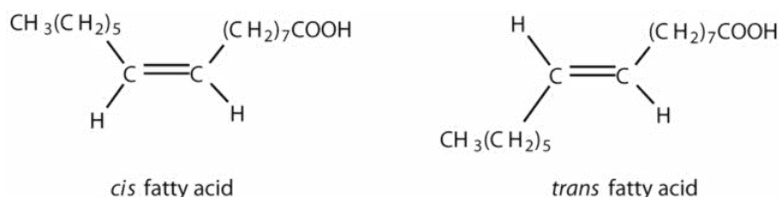


Table 1.3.3.1 lists some common fatty acids and one important source for each. The atoms or groups around the double bonds in unsaturated fatty acids can be arranged in either the *cis* or *trans* isomeric form. Naturally occurring fatty acids are generally in the *cis* configuration.

Table 1.3.3.1 Some Common Fatty Acids Found in Natural Fats.

Name	Abbreviated Structural Formula	Condensed Structural Formula	Melting Point (°C)	Source
lauric acid	$\text{C}_{11}\text{H}_{23}\text{COOH}$	$\text{CH}_3(\text{CH}_2)_{10}\text{COOH}$	44	palm kernel oil
myristic acid	$\text{C}_{13}\text{H}_{27}\text{COOH}$	$\text{CH}_3(\text{CH}_2)_{12}\text{COOH}$	58	oil of nutmeg
palmitic acid	$\text{C}_{15}\text{H}_{31}\text{COOH}$	$\text{CH}_3(\text{CH}_2)_{14}\text{COOH}$	63	palm oil
palmitoleic acid	$\text{C}_{15}\text{H}_{29}\text{COOH}$	$\text{CH}_3(\text{CH}_2)_5\text{CH}=\text{CH}(\text{CH}_2)_7\text{COOH}$	0.5	macadamia oil
stearic acid	$\text{C}_{17}\text{H}_{35}\text{COOH}$	$\text{CH}_3(\text{CH}_2)_{16}\text{COOH}$	70	cocoa butter
oleic acid	$\text{C}_{17}\text{H}_{33}\text{COOH}$	$\text{CH}_3(\text{CH}_2)_7\text{CH}=\text{CH}(\text{CH}_2)_7\text{COOH}$	16	olive oil
linoleic acid	$\text{C}_{17}\text{H}_{31}\text{COOH}$	$\text{CH}_3(\text{CH}_2)_3(\text{CH}_2\text{CH}=\text{CH})_2(\text{CH}_2)_7\text{COOH}$	-5	canola oil
α -linolenic acid	$\text{C}_{17}\text{H}_{29}\text{COOH}$	$\text{CH}_3(\text{CH}_2\text{CH}=\text{CH})_3(\text{CH}_2)_7\text{COOH}$	-11	flaxseed
arachidonic acid	$\text{C}_{19}\text{H}_{31}\text{COOH}$	$\text{CH}_3(\text{CH}_2)_4(\text{CH}_2\text{CH}=\text{CH})_4(\text{CH}_2)_2\text{COOH}$	-50	liver

Two polyunsaturated fatty acids—linoleic and α -linolenic acids—are termed essential fatty acids because humans must obtain them from their diets. Both substances are required for normal growth and development, but the human body does not synthesize them. The body uses linoleic acid to synthesize many of the other unsaturated fatty acids, such as arachidonic acid, a precursor for the synthesis of prostaglandins. In addition, the essential fatty acids are necessary for the efficient transport and metabolism of cholesterol. The average daily diet should contain about 4–6 g of the essential fatty acids.

Fats and oils are the most abundant lipids in nature. They provide energy for living organisms, insulate body organs, and transport fat-soluble vitamins through the blood. Although we often draw the carbon atoms in a straight line, they actually have more of a zigzag configuration (Figure 1.3.3.2a). Viewed as a whole, however, the saturated fatty acid molecule is relatively straight (Figure 1.3.3.2b). Such molecules pack closely together into a crystal lattice, maximizing the strength of dispersion forces and causing fatty acids and the fats derived from them to have relatively high melting points. In contrast, each *cis* carbon-to-carbon double bond in an unsaturated fatty acid produces a pronounced bend in the molecule, so that these molecules do not stack neatly. As a result, the intermolecular attractions of unsaturated fatty acids (and unsaturated fats) are weaker, causing these substances to have lower melting points. Most are liquids at room temperature.

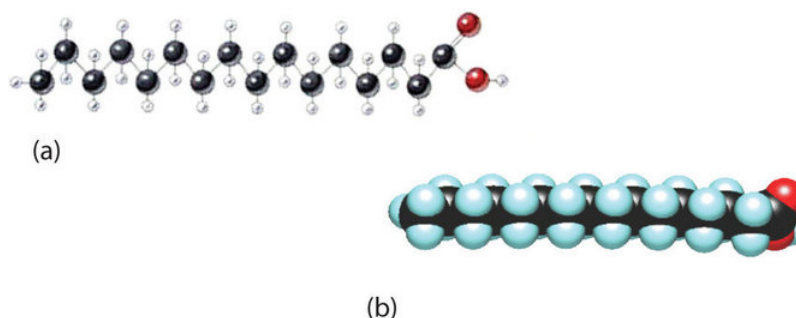
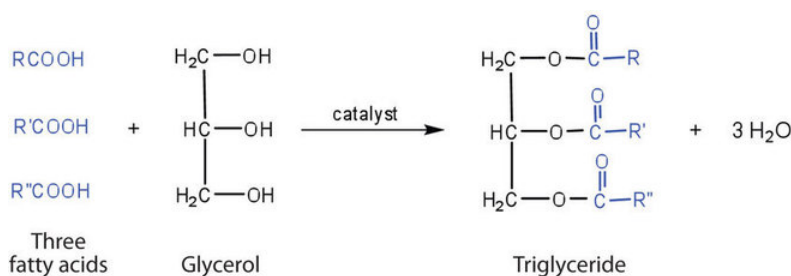


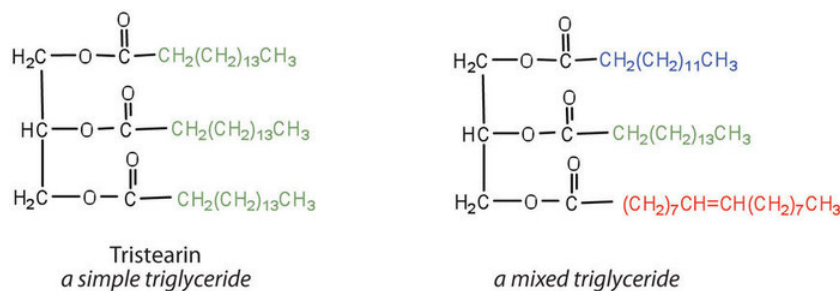
Figure 1.3.3.2 The Structure of Saturated Fatty Acids. (a) There is a zigzag pattern formed by the carbon-to-carbon single bonds in the ball-and-stick model of a palmitic acid molecule. (b) A space-filling model of palmitic acid shows the overall straightness of a saturated fatty acid molecule.

Structures of Fats and Oils

Fats and oils are called triglycerides (or *triacylglycerols*) because they are esters composed of three fatty acid units joined to *glycerol*, a trihydroxy alcohol:



If all three OH groups on the glycerol molecule are esterified with the same fatty acid, the resulting ester is called a *simple triglyceride*. Although simple triglycerides have been synthesized in the laboratory, they rarely occur in nature. Instead, a typical triglyceride obtained from naturally occurring fats and oils contains two or three different fatty acid components and is thus termed a *mixed triglyceride*.



A triglyceride is called a fat if it is a solid at 25°C; it is called an oil if it is a liquid at that temperature. These differences in melting points reflect differences in the degree of unsaturation and number of carbon atoms in the constituent fatty acids. Triglycerides obtained from animal sources are usually solids, while those of plant origin are generally oils. Therefore, we commonly speak of animal fats and vegetable oils.

No single formula can be written to represent the naturally occurring fats and oils because they are highly complex mixtures of triglycerides in which many different fatty acids are represented. Table 1.3.3.2 shows the fatty acid compositions of some common fats and oils. The composition of any given fat or oil can vary depending on the plant or animal species it comes from as well as on dietetic and climatic factors. To cite just one example, lard from corn-fed hogs is more highly saturated than lard from peanut-fed hogs. Palmitic acid is the most abundant of the saturated fatty acids, while oleic acid is the most abundant unsaturated fatty acid.

Table 1.3.3.2 Average Fatty Acid Composition of Some Common Fats and Oils (%)*.

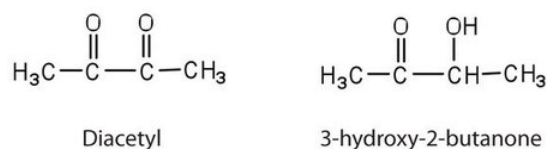
Lauric	Myristic	Palmitic	Stearic	Oleic	Linoleic	Linolenic

	Lauric	Myristic	Palmitic	Stearic	Oleic	Linoleic	Linolenic
Fats							
butter (cow)	3	11	27	12	29	2	1
tallow		3	24	19	43	3	1
lard		2	26	14	44	10	
Oils							
canola oil			4	2	62	22	10
coconut oil [†]	47	18	9	3	6	2	
corn oil			11	2	28	58	1
olive oil			13	3	71	10	1
peanut oil			11	2	48	32	
soybean oil			11	4	24	54	7
*Totals less than 100% indicate the presence of fatty acids with fewer than 12 carbon atoms or more than 18 carbon atoms.							
[†] Coconut oil is highly saturated. It contains an unusually high percentage of the low-melting C ₈ , C ₁₀ , and C ₁₂ saturated fatty acids.							

Terms such as **saturated fat** or **unsaturated oil** are often used to describe the fats or oils obtained from foods. **Saturated fats** contain a high proportion of saturated fatty acids, while **unsaturated oils** contain a high proportion of unsaturated fatty acids. The high consumption of saturated fats is a factor, along with the high consumption of cholesterol, in increased risks of heart disease.

Physical Properties of Fats and Oils

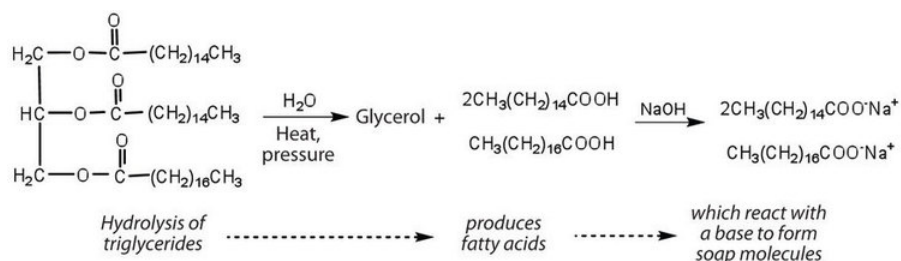
Contrary to what you might expect, *pure* fats and oils are colorless, odorless, and tasteless. The characteristic colors, odors, and flavors that we associate with some of them are imparted by foreign substances that are lipid soluble and have been absorbed by these lipids. For example, the yellow color of butter is due to the presence of the pigment carotene; the taste of butter comes from two compounds—diacetyl and 3-hydroxy-2-butanone—produced by bacteria in the ripening cream from which the butter is made.



Fats and oils are lighter than water, having densities of about 0.8 g/cm³. They are poor conductors of heat and electricity and therefore serve as excellent insulators for the body, slowing the loss of heat through the skin.

Chemical Reactions of Fats and Oils

Fats and oils can participate in a variety of chemical reactions—for example, because triglycerides are esters, they can be hydrolyzed in the presence of an acid, a base, or specific enzymes known as lipases. The hydrolysis of fats and oils in the presence of a base is used to make soap and is called saponification. Today most soaps are prepared through the hydrolysis of triglycerides (often from tallow, coconut oil, or both) using water under high pressure and temperature [700 lb/in² (~50 atm or 5,000 kPa) and 200°C]. Sodium carbonate or sodium hydroxide is then used to convert the fatty acids to their sodium salts (soap molecules):



Iodine Value

The **iodine value** (or **iodine adsorption value** or **iodine number** or **iodine index**, commonly abbreviated as **IV**) in chemistry is the mass of iodine in grams that is consumed by 100 grams of a chemical substance. Iodine numbers are often used to determine the amount of unsaturation in fats, oils and waxes. In fatty acids, unsaturation occurs mainly as double bonds which are very reactive towards halogens, the iodine in this case. Thus, the higher the iodine value, the more unsaturations are present in the fat. It can be seen from the table that coconut oil is very saturated, which means it is good for making soap. On the other hand, linseed oil is highly unsaturated, which makes it a drying oil, well suited for making oil paints.

Table 1.3.3.1 Iodine Numbers of Common Fats and Oils. Source Wikipedia

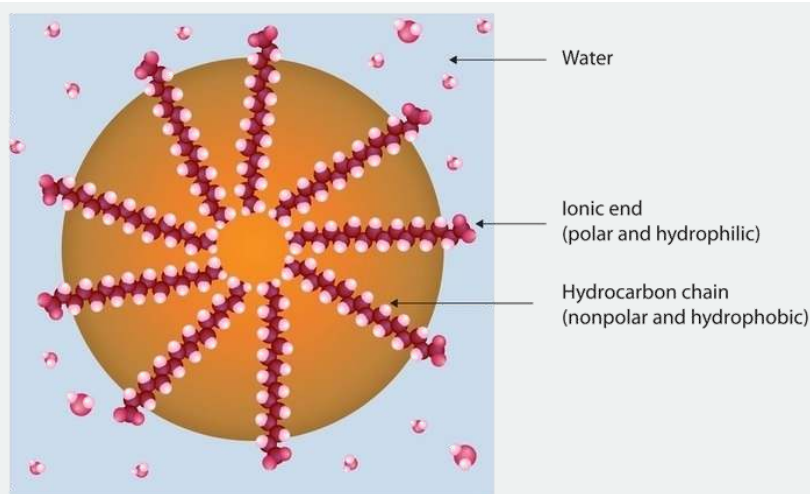
Fat	Iodine Value (g/100g)
Beef tallow	42-48
Butter	25-42
Canola Oil	110-126
Coconut Oil	6-11
Fish oil	190-205
Linseed Oil	170-204
Olive Oil	75-94
Safflower Oil	135-150
Walnut Oil	132-162

Looking Closer: Soaps

Ordinary soap is a mixture of the sodium salts of various fatty acids, produced in one of the oldest organic syntheses practiced by humans (second only to the fermentation of sugars to produce ethyl alcohol). Both the Phoenicians (600 BCE) and the Romans made soap from animal fat and wood ash. Even so, the widespread production of soap did not begin until the 1700s.

Soap was traditionally made by treating molten lard or tallow with a slight excess of alkali in large open vats. The mixture was heated, and steam was bubbled through it. After saponification was completed, the soap was precipitated from the mixture by the addition of sodium chloride (NaCl), removed by filtration, and washed several times with water. It was then dissolved in water and reprecipitated by the addition of more NaCl. The glycerol produced in the reaction was also recovered from the aqueous wash

solutions.



does little to remove them. Soap removes them, however, because soap molecules have a dual nature. One end, called the *head*, carries an ionic charge (a carboxylate anion) and therefore dissolves in water; the other end, the *tail*, has a hydrocarbon structure and dissolves in oils. The hydrocarbon tails dissolve in the oil; the ionic heads remain in the aqueous phase, and the soap breaks the oil into tiny soap-enclosed droplets called *micelles*, which disperse throughout the solution. The droplets repel each other because of their charged surfaces and do not coalesce. With the oil no longer “gluing” the dirt to the soiled surface (skin, cloth, dish), the soap-enclosed dirt can easily be rinsed away.

Pumice or sand is added to produce scouring soap, while ingredients such as perfumes or dyes are added to produce fragrant, colored soaps. Blowing air through molten soap produces a floating soap. Soft soaps, made with potassium salts, are more expensive but produce a finer lather and are more soluble. They are used in liquid soaps, shampoos, and shaving creams.

Dirt and grime usually adhere to skin, clothing, and other surfaces by combining with body oils, cooking fats, lubricating greases, and similar substances that act like glues. Because these substances are not miscible in water, washing with water alone

Summary

- Fatty acids are carboxylic acids that are the structural components of many lipids.
- Saturated fatty acids contain no carbon-to-carbon double bonds, monounsaturated fatty acids contain one carbon-to-carbon double bond, and polyunsaturated fatty acids contain two or more carbon-to-carbon double bonds.
- Fats and oils are composed of molecules known as triglycerides, which are esters composed of three fatty acid units linked to glycerol.
- Fats and oils can participate in a variety of chemical reactions—for example, because triglycerides are esters, they can be hydrolyzed in the presence of an acid, a base, or specific enzymes known as lipases.
- The hydrolysis of fats and oils in the presence of a base is used to make soap and is called saponification.
- Animal fats and oils which are made up mostly of saturated fatty acids have low iodine values (numbers), while those oils with high degree of unsaturation (with more C=C bonds) have high iodine values.

Contributors and Attributions

- Libretext: The Basics of GOB Chemistry (Ball et al.)
- Wikipedia
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1.3.4: Proteins- Polymers of Amino Acids

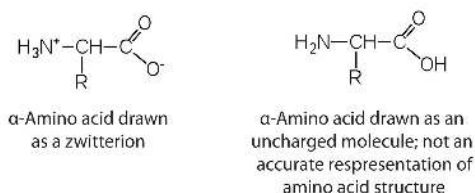
Learning Objectives

- Identify different amino acids.
- Describe how short chain proteins (polypeptides) are formed from amino acids.

Proteins may be defined as compounds of high molar mass consisting largely or entirely of chains of amino acids. Their masses range from several thousand to several million daltons (Da). In addition to carbon, hydrogen, and oxygen atoms, all proteins contain nitrogen and sulfur atoms, and many also contain phosphorus atoms and traces of other elements. Proteins serve a variety of roles in living organisms and are often classified by these biological roles. Muscle tissue is largely protein, as are skin and hair. Proteins are present in the blood, in the brain, and even in tooth enamel. Each type of cell in our bodies makes its own specialized proteins, as well as proteins common to all or most cells. We begin our study of proteins by looking at the properties and reactions of amino acids, which is followed by a discussion of how amino acids link covalently to form peptides and proteins. We end the chapter with a discussion of enzymes—the proteins that act as catalysts in the body.

The proteins in all living species, from bacteria to humans, are constructed from the same set of 20 amino acids, so called because each contains an amino group attached to a carboxylic acid. The amino acids in proteins are α -amino acids, which means the amino group is attached to the α -carbon of the carboxylic acid. Humans can synthesize only about half of the needed amino acids; the remainder must be obtained from the diet and are known as essential amino acids. However, two additional amino acids have been found in limited quantities in proteins: Selenocysteine was discovered in 1986, while pyrrolysine was discovered in 2002.

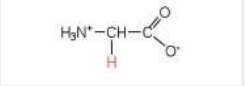
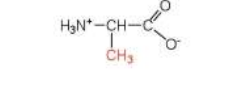
The amino acids are colorless, nonvolatile, crystalline solids, melting and decomposing at temperatures above 200°C. These melting temperatures are more like those of inorganic salts than those of amines or organic acids and indicate that the structures of the amino acids in the solid state and in neutral solution are best represented as having both a negatively charged group and a positively charged group. Such a species is known as a zwitterion.



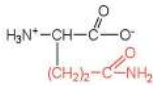
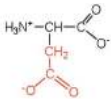
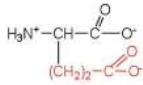
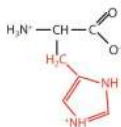
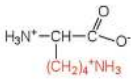
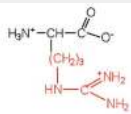
Classification

In addition to the amino and carboxyl groups, amino acids have a side chain or R group attached to the α -carbon. Each amino acid has unique characteristics arising from the size, shape, solubility, and ionization properties of its R group. As a result, the side chains of amino acids exert a profound effect on the structure and biological activity of proteins. Although amino acids can be classified in various ways, one common approach is to classify them according to whether the functional group on the side chain at neutral pH is nonpolar, polar but uncharged, negatively charged, or positively charged. The structures and names of the 20 amino acids, their one- and three-letter abbreviations, and some of their distinctive features are given in Table 1.3.4.1.

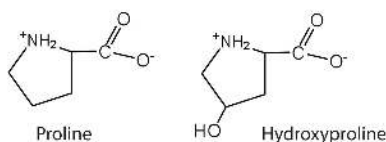
Table 1.3.4.1: Common Amino Acids Found in Proteins

Common Name	Abbreviation	Structural Formula (at pH 6)	Molar Mass	Distinctive Feature
Amino acids with a nonpolar R group				
glycine	gly (G)		75	the only amino acid lacking a chiral carbon
alanine	ala (A)		89	—

Common Name	Abbreviation	Structural Formula (at pH 6)	Molar Mass	Distinctive Feature
valine	val (V)		117	a branched-chain amino acid
leucine	leu (L)		131	a branched-chain amino acid
isoleucine	ile (I)		131	an essential amino acid because most animals cannot synthesize branched-chain amino acids
phenylalanine	phe (F)		165	also classified as an aromatic amino acid
tryptophan	trp (W)		204	also classified as an aromatic amino acid
methionine	met (M)		149	side chain functions as a methyl group donor
proline	pro (P)		115	contains a secondary amine group; referred to as an α -imino acid
Amino acids with a polar but neutral R group				
serine	ser (S)		105	found at the active site of many enzymes
threonine	thr (T)		119	named for its similarity to the sugar threose
cysteine	cys (C)		121	oxidation of two cysteine molecules yields <i>cystine</i>
tyrosine	tyr (Y)		181	also classified as an aromatic amino acid
asparagine	asn (N)		132	the amide of aspartic acid

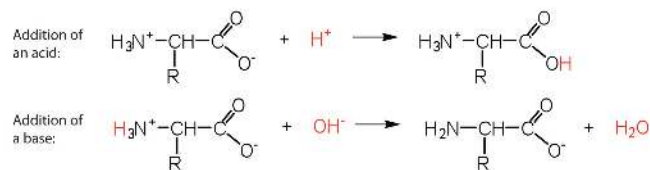
Common Name	Abbreviation	Structural Formula (at pH 6)	Molar Mass	Distinctive Feature
glutamine	gln (Q)		146	the amide of glutamic acid
Amino acids with a negatively charged R group				
aspartic acid	asp (D)		132	carboxyl groups are ionized at physiological pH; also known as aspartate
glutamic acid	glu (E)		146	carboxyl groups are ionized at physiological pH; also known as glutamate
Amino acids with a positively charged R group				
histidine	his (H)		155	the only amino acid whose R group has a pK _a (6.0) near physiological pH
lysine	lys (K)		147	—
arginine	arg (R)		175	almost as strong a base as sodium hydroxide

The first amino acid to be isolated was asparagine in 1806. It was obtained from protein found in asparagus juice (hence the name). Glycine, the major amino acid found in gelatin, was named for its sweet taste (Greek *glykys*, meaning “sweet”). In some cases an amino acid found in a protein is actually a derivative of one of the common 20 amino acids (one such derivative is hydroxyproline). The modification occurs *after* the amino acid has been assembled into a protein.



Zwitterions

The structure of an amino acid allows it to act as both an acid and a base. An amino acid has this ability because at a certain pH value (different for each amino acid) nearly all the amino acid molecules exist as zwitterions. If acid is added to a solution containing the zwitterion, the carboxylate group captures a hydrogen (H^+) ion, and the amino acid becomes positively charged. If base is added, ion removal of the H^+ ion from the amino group of the zwitterion produces a negatively charged amino acid. In both circumstances, the amino acid acts to maintain the pH of the system—that is, to remove the added acid (H^+) or base (OH^-) from solution.



The Peptide Bond: Peptides and Proteins

Two or more amino acids can join together into chains called peptides. Previously, we discussed the reaction between ammonia and a carboxylic acid to form an amide. In a similar reaction, the amino group on one amino acid molecule reacts with the carboxyl group on another, releasing a molecule of water and forming an amide linkage as shown in Figure 1.3.4.1

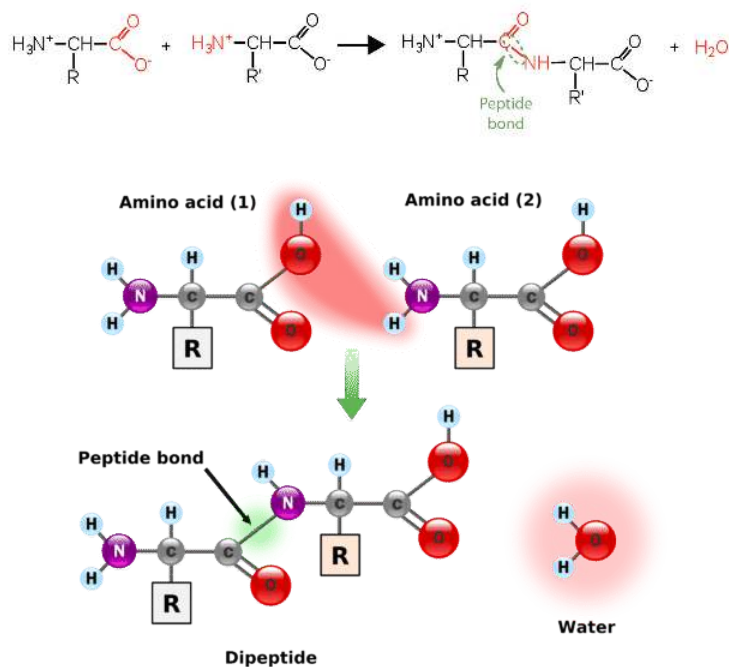
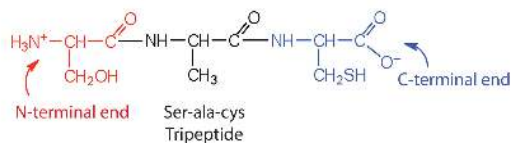


Figure 1.3.4.1 Amino acids undergo condensation to form a molecule called a dipeptide. The C—N bond is called a peptide bond.

An amide bond joining two amino acid units is called a peptide bond. Note that the product molecule still has a reactive amino group on the left and a reactive carboxyl group on the right. These can react with additional amino acids to lengthen the peptide. The process can continue until thousands of units have joined, resulting in large proteins.

A chain consisting of only two amino acid units is called a *dipeptide*; a chain consisting of three is a *tripeptide*. By convention, peptide and protein structures are depicted with the amino acid whose amino group is free (the N-terminal end) on the left and the amino acid with a free carboxyl group (the C-terminal end) to the right.



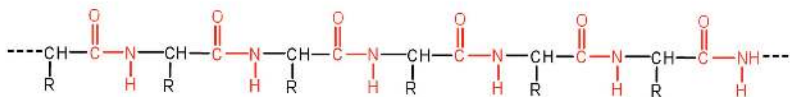
The general term *peptide* refers to an amino acid chain of unspecified length. However, chains of about 50 amino acids or more are usually called proteins or polypeptides. In its physiologically active form, a protein may be composed of one or more polypeptide chains.

Peptide cells in our bodies have an intricate mechanism for the manufacture of proteins. Humans have to use other techniques in order to synthesize the same proteins in a lab. The chemistry of peptide synthesis is complicated. Both active groups on an amino acid can react and the amino acid sequence must be a specific one in order for the protein to function. Robert Merrifield developed

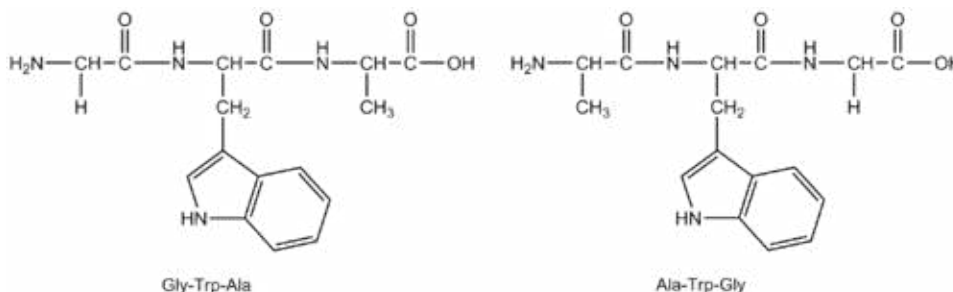
the first synthetic approach for making proteins in the lab, a manual approach which was lengthy and tedious (and, he won the Nobel Prize in Chemistry in 1984 for his work). Today, however, automated systems can crank out a peptide in a very short period of time.

The Sequence of Amino Acids

The particular sequence of amino acids in a longer chain is called an amino acid sequence. By convention, the amino acid sequence is listed in the order such that the free amine group is on the left end of the molecule and the free carboxyl group is on the right end of the molecule.



For example, suppose that a sequence of the amino acids glycine, tryptophan, and alanine is formed with the free amine group as part of the glycine and the free carboxyl group as part of the alanine. The amino acid sequence can be easily written using the abbreviations as Gly-Trp-Ala. This is a different sequence from Ala-Trp-Gly because the free amine and carboxyl groups would be on different amino acids in that case.



Bradykinin

For peptides and proteins to be physiologically active, it is not enough that they incorporate certain amounts of specific amino acids. The order, or *sequence*, in which the amino acids are connected is also of critical importance. Bradykinin is a nine-amino acid peptide (Figure 1.3.4.2) produced in the blood that has the following amino acid sequence:

arg-pro-pro-gly-phe-ser-pro-phe-arg

This peptide lowers blood pressure, stimulates smooth muscle tissue, increases capillary permeability, and causes pain. When the order of amino acids in bradykinin is reversed,

arg-phe-pro-ser-phe-gly-pro-pro-arg

the peptide resulting from this synthesis shows none of the activity of bradykinin.

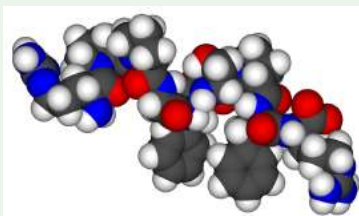


Figure 1.3.4.2 Space-filling model of bradykinin. (Public Domain; Fvasconcellos)

Just as millions of different words are spelled with our 26-letter English alphabet, millions of different proteins are made with the 20 common amino acids. However, just as the English alphabet can be used to write gibberish, amino acids can be put together in the *wrong sequence* to produce nonfunctional proteins. Although the correct sequence is ordinarily of utmost

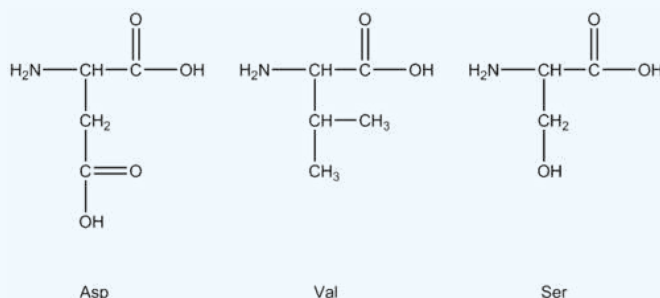
importance, it is not always absolutely required. Just as you can sometimes make sense of incorrectly spelled English words, a protein with a small percentage of “incorrect” amino acids may continue to function. However, it rarely functions as well as a protein having the correct sequence. There are also instances in which seemingly minor errors of sequence have disastrous effects. For example, in some people, every molecule of hemoglobin (a protein in the blood that transports oxygen) has a single incorrect amino acid unit out of about 300 (a single valine replaces a glutamic acid). That “minor” error is responsible for sickle cell anemia, an inherited condition that usually is fatal.

✓ Example 1.3.4.1

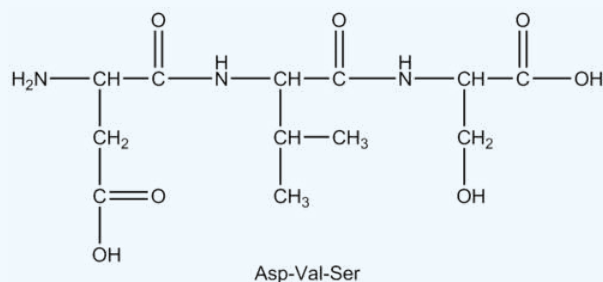
Draw the polypeptide Asp-Val-Ser.

Solution

1. Identify the structures of each of the three given amino acids and draw them in the same order as given in the name.



2. Leaving the order the same, connect the amino acids to one another by forming peptide bonds. Note that the order given in the name is the same way the amino acids are connected in the molecule. The first one listed is always the N-terminus of the polypeptide.



✓ Example 1.3.4.2

List all of the possible polypeptides that can be formed from cysteine (Cys), leucine (Leu), and arginine (Arg).

Solution

Although there are only three amino acids, the order in which they are bonded changes the identity, properties, and function of the resulting polypeptide. There are six possible polypeptides formed from these three amino acids.

Cys-Leu-Arg

Cys-Arg-Leu

Leu-Cys-Arg

Leu-Arg-Cys

Arg-Cys-Leu

Arg-Leu-Cys

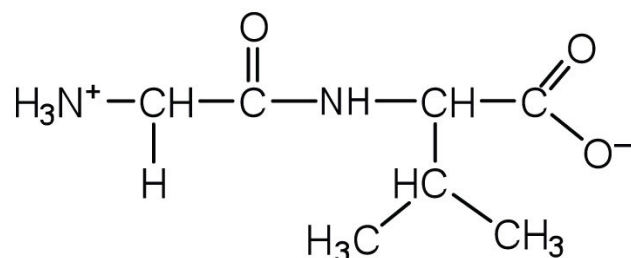
✓ Exercise 1.3.4.1

Draw the structure for each peptide.

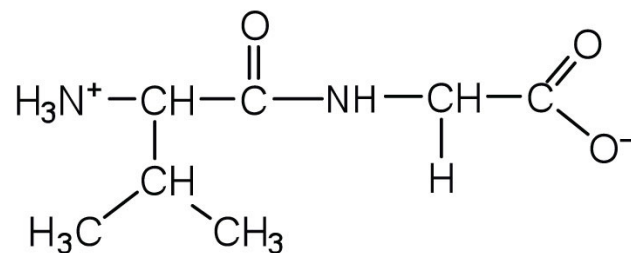
- gly-val
- val-gly

Answers

a.



b.



Summary

- The amino group of one amino acid can react with the carboxyl group on another amino acid to form a peptide bond that links the two amino acids together.
- Additional amino acids can be added on through the formation of addition peptide (amide) bonds.
- A chain consisting of only two amino acid units is called a *dipeptide*; a chain consisting of three is a *tripeptide*.
- Chains of about 50 amino acids or more are usually called proteins or polypeptides.
- A sequence of amino acids in a peptide or protein is written with the N-terminal amino acid first and the C-terminal amino acid at the end (writing left to right).
- The order, or *sequence*, in which the amino acids are connected is also of critical importance in order for a peptide or protein to be physiologically active.

Contributors and Attributions

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1.4: Macro- and Micronutrients

Building from the last section that looked at the structures of macro-nutrients, this section will focus on how we break down macro-nutrients to use for different purposes in our body. It will also briefly examine the structure and function of micro-nutrients.

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1.4.1: Carbohydrates in the Diet

Learning Objectives

- Describe the metabolism of carbohydrates.
- Know the source and function of common carbohydrates in the diet.

Carbohydrates are sugars and sugar derivatives whose formulas can be written in the general form: $C_x(H_2O)_y$. (The subscripts x and y are whole numbers.) Some typical carbohydrates are sucrose (ordinary cane sugar), $C_{12}H_{22}O_{11}$; glucose (dextrose), $C_6H_{12}O_6$; fructose (fruit sugar), $C_6H_{12}O_6$; and ribose, $C_5H_{10}O_5$. Since the atom ratio H/O is 2/1 in each formula, these compounds were originally thought to be hydrates of carbon, hence their general name.

In scientific literature, the term "carbohydrate" has many synonyms, like "sugar" (in the broad sense), "saccharide", "ose", "glucide", "hydrate of carbon" or "polyhydroxy compounds with aldehyde or ketone". Some of these terms, specially "carbohydrate" and "sugar", are also used with other meanings.

In food science and in many informal contexts, the term "carbohydrate" often means any food that is particularly rich in the complex carbohydrate starch (such as cereals, bread and pasta) or simple carbohydrates, such as sugar (found in candy, jams, and desserts).

Carbohydrates may be classified according to their degree of polymerization, and may be divided initially into three principal groups, namely sugars, oligosaccharides and polysaccharides as shown in Table 1.4.1.1.

Table 1.4.1.1 The Major Dietary Carbohydrates. Source: Wikipedia

Class (DP*)	Subgroup	Components
Sugars (1-2)	Monosaccharides	Glucose, galactose, fructose, xylose
	Disaccharides	Sucrose, lactose, maltose, trehalose
	Polyols	Sorbitol, mannitol
Oligosaccharides (3-9)	Malto-oligosaccharides	Maltodextrins
	Other oligosaccharides	Raffinose, stachyose, fructo-oligosaccharides
Polysaccharides (>9)	Starch	Amylose, amylopectin, modified starches
	Non-starch polysaccharides	Glycogen, Cellulose, Hemicellulose, Pectins, Hydrocolloids

DP * = Degree of polymerization

Digestion of Carbohydrates

The human body breaks down complex carbohydrates into **glucose**. Glucose in the blood (often referred to as "blood sugar") is the **primary energy source** for the body. Sugars provide calories, or "energy," for the body. Each gram of sugar provides **4 calories**. Glucose can be used immediately or stored in the liver and muscles for later use.

Carbohydrate digestion begins in the mouth (Figure 1.4.1.1) where salivary α -amylase attacks the α -glycosidic linkages in starch, the main carbohydrate ingested by humans. Cleavage of the glycosidic linkages produces a mixture of dextrins, maltose, and glucose. The α -amylase mixed into the food remains active as the food passes through the esophagus, but it is rapidly inactivated in the acidic environment of the stomach.

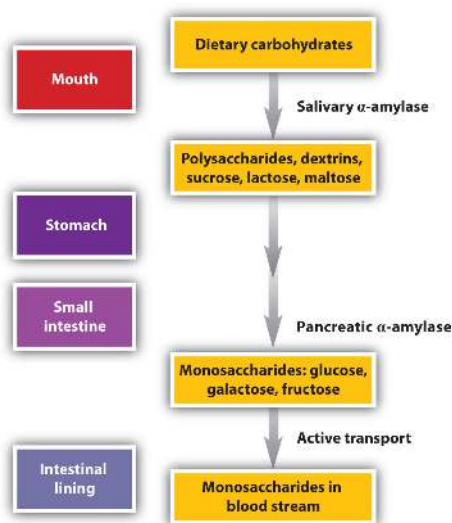


Figure 1.4.1.1 The Principal events and sites of carbohydrate digestion.

The primary site of carbohydrate digestion is the small intestine. The secretion of α -amylase in the small intestine converts any remaining starch molecules, as well as the dextrins, to maltose. Maltose is then cleaved into two glucose molecules by maltase. Disaccharides such as sucrose and lactose are not digested until they reach the small intestine, where they are acted on by sucrase and lactase, respectively. The major products of the complete hydrolysis of disaccharides and polysaccharides are three monosaccharide units: glucose, fructose, and galactose. These are absorbed through the wall of the small intestine into the bloodstream.

Fuel for the Brain

The brain is a marvelous organ. And it's a hungry one, too. The major fuel for the brain is the carbohydrate glucose. The average adult brain represents about 2% of our body's weight, but uses 25% of the glucose in the body. Moreover, specific areas of the brain use glucose at different rates. If you are concentrating hard (taking a test, for example), certain parts of the brain need a lot of extra glucose while other parts of the brain only use their normal amount. Something to think about.

Some foods that are high in carbohydrates include bread, pasta, and potatoes (Figure 1.4.1.2). Because carbohydrates are easily digested, athletes often rely on carbohydrate rich foods to enable a high level of performance.



Figure 1.4.1.2 Foods that serve as carbohydrate sources.

Common Monosaccharides and Disaccharides

Monosaccharides and disaccharides commonly found in our diets are listed in Table 1.4.1.3. Although a variety of monosaccharides are found in living organisms, three hexoses are particularly abundant: D-glucose, D-galactose, and D-fructose (Figure 1.4.1.3). Glucose and galactose are both aldohexoses, while fructose is a ketohexose.

Table 1.4.1.2. Monosaccharides and disaccharides. Source: US FDA

Simple sugars (monosaccharides) are small enough to be absorbed directly into the bloodstream. They include:	Sugars that contain two molecules of sugar linked together (disaccharides) are broken down in your body into single sugars. They include:
Fructose	Sucrose (table sugar) = glucose + fructose
Galactose	Lactose (milk sugar) = glucose + galactose
Glucose	Maltose (malt sugar) = glucose + glucose

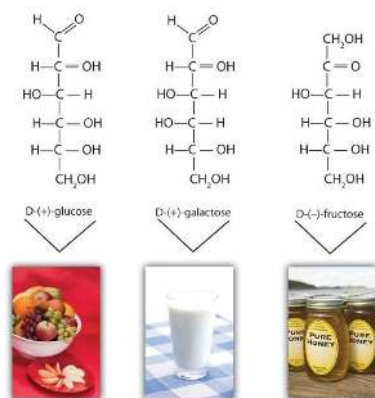


Figure 1.4.1.3 Structures of three important hexoses. Each hexose is pictured with a food source in which it is commonly found. Source: Photos © Thinkstock.

Glucose

D-Glucose, generally referred to as simply glucose, is the most abundant sugar found in nature; most of the carbohydrates we eat are eventually converted to it in a series of biochemical reactions that produce energy for our cells. It is also known by three other names: *dextrose*, from the fact that it rotates plane-polarized light in a clockwise (dextrorotatory) direction; *corn sugar* because in the United States cornstarch is used in the commercial process that produces glucose from the hydrolysis of starch; and *blood sugar* because it is the carbohydrate found in the circulatory system of animals. Normal blood sugar values range from 70 to 105 mg glucose/dL plasma, and normal urine may contain anywhere from a trace to 20 mg glucose/dL urine.

Galactose

D-Galactose does not occur in nature in the uncombined state. It is released when lactose, a disaccharide found in milk, is hydrolyzed. The galactose needed by the human body for the synthesis of lactose is obtained by the metabolic conversion of D-glucose to D-galactose. Galactose is also an important constituent of the glycolipids that occur in the brain and the myelin sheath of nerve cells. For this reason it is also known as *brain sugar*. The structure of D-galactose is shown in Figure 1.4.1.3 Notice that the configuration differs from that of glucose only at the fourth carbon atom.

Fructose

D-Fructose, also shown in Figure 1.4.1.3 is the most abundant ketohexose. Note that from the third through the sixth carbon atoms, its structure is the same as that of glucose. It occurs, along with glucose and sucrose, in honey (which is 40% fructose) and sweet fruits. Fructose (from the Latin *fructus*, meaning "fruit") is also referred to as *levulose* because it has a specific rotation that is strongly levorotatory (-92.4°). It is the sweetest sugar, being 1.7 times sweeter than sucrose, although many nonsugars are several hundred or several thousand times as sweet (Table 1.4.1.1).

Sucrose

Sucrose, probably the largest-selling pure organic compound in the world, is known as *beet sugar*, *cane sugar*, *table sugar*, or simply *sugar*. Most of the sucrose sold commercially is obtained from sugar cane and sugar beets (whose juices are 14%–20% sucrose) by evaporation of the water and recrystallization. The dark brown liquid that remains after the recrystallization of sugar is sold as molasses.

Maltose

Maltose occurs to a limited extent in sprouting grain. It is formed most often by the partial hydrolysis of starch and glycogen. In the manufacture of beer, maltose is liberated by the action of malt (germinating barley) on starch; for this reason, it is often referred to as *malt sugar*. Maltose is about 30% as sweet as sucrose. The human body is unable to metabolize maltose or any other disaccharide directly from the diet because the molecules are too large to pass through the cell membranes of the intestinal wall. Therefore, an ingested disaccharide must first be broken down by hydrolysis into its two constituent monosaccharide units.

In the body, such hydrolysis reactions are catalyzed by enzymes such as *maltase*.

Lactose

Lactose is known as *milk sugar* because it occurs in the milk of humans, cows, and other mammals. In fact, the natural synthesis of lactose occurs only in mammary tissue, whereas most other carbohydrates are plant products. Human milk contains about 7.5% lactose, and cow's milk contains about 4.5%. This sugar is one of the lowest ranking in terms of sweetness, being about one-sixth as sweet as sucrose. Lactose is produced commercially from whey, a by-product in the manufacture of cheese. It is important as an infant food and in the production of penicillin.

Many adults and some children suffer from a deficiency of lactase. These individuals are said to be lactose intolerant because they cannot digest the lactose found in milk. A more serious problem is the genetic disease galactosemia, which results from the absence of an enzyme needed to convert galactose to glucose. Certain bacteria can metabolize lactose, forming lactic acid as one of the

products. This reaction is responsible for the “souring” of milk.

The different disaccharides and the monosaccharides components are illustrated in Figure 1.4.1.4 below.

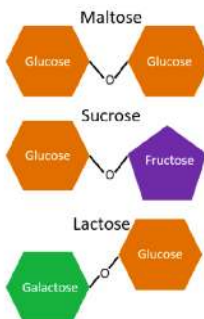


Figure 1.4.1.4 The three disaccharides.

Each of these disaccharides contains glucose and all the reactions are dehydration reactions. Also notice the difference in the bond structures. Maltose and sucrose have alpha-bonds, which are depicted as v-shaped above. You might hear the term glycosidic used in some places to describe bonds between sugars. A **glycoside** is a sugar, so **glycosidic** is referring to a sugar bond. Lactose, on the other hand, contains a beta-bond. We need a special enzyme, **lactase**, to break this bond, and the absence of lactase activity leads to lactose intolerance.

Naturally Occurring and Added Sugars

Sugars are found *naturally* in many nutritious foods and beverages and are also added to foods and beverages for taste, texture, and preservation.

Naturally occurring sugars are found in a variety of foods, including:	Added sugars are often found in foods low in other nutrients, including:
- Dairy products - Fruit (fresh, frozen, dried, and canned in 100% fruit juice) 100% fruit and vegetable juice - Vegetables	- Dairy desserts (such as ice cream, other frozen desserts, and puddings) - Grain-based desserts (such as brownies, cakes, cookies, doughnuts, pastries, pies, and sweet rolls) - Sugar-sweetened beverages (such as energy drinks, flavored waters, fruit drinks, soft drinks, sports drinks, and sweetened coffee and tea) - Sweets (such as candies, jams, sweet toppings, and syrups)

The relative sweetness of the different sugars previously discussed are given in Table 1.4.1.3

Table 1.4.1.3: The Relative Sweetness of Some Sugars (Sucrose = 100)

Compound	Relative Sweetness
lactose	16
maltose	32
glucose	74
sucrose	100
fructose	173

High-Fructose Corn Syrup

Figure 1.4.1.5 U.S. per capita sugar and sweetener consumption

Opponents claim that high-fructose corn syrup is contributing to the rise in obesity rates. As a result, some manufacturers have started releasing products made with natural sugar. You can read about this trend in the following New York Times article in the link below. Also, manufacturers tried to rebrand high-fructose corn syrup as corn sugar to get around the negative perception of the name. But the FDA rejected the Corn Refiners Association request to change the name officially to corn sugar as described in the second link. The last link is a video made by the American Chemical Society that gives some background on how HFCS is produced and how it compares to sucrose.

Links and Video

Links

Sugar is back on labels, this time as a selling point - http://www.nytimes.com/2009/03/21/dining/21sugar.html?_r=1&ref=nutrition

No new name for high-fructose corn syrup - http://well.blogs.nytimes.com/2012/05/31/no-new-name-for-high-fructose-corn-syrup/?_r=0

Video

Sugar vs. High Fructose Corn Syrup - What's the Difference? - <https://www.youtube.com/watch?v=fXMvregmU1g>

Complex Carbohydrates: Oligosaccharides and Polysaccharides

An **oligosaccharide**, from the Greek *oligos*, "a few", and *sáchar*, "sugar") is a saccharide polymer containing a small number (typically three to ten) of monosaccharides (simple sugars). Oligosaccharides are a component of fiber from plant tissue. Fructooligosaccharides (FOS) and inulin (Figure 1.4.1.6) are present in Jerusalem artichoke, burdock, chicory, leeks, onions, and asparagus. Inulin is a significant part of the daily diet of most of the world's population. FOS can also be synthesized by enzymes of the fungus *Aspergillus niger* acting on sucrose. Galactooligosaccharide (GOS) is naturally found in soybeans and can be synthesized from lactose. FOS, GOS, and inulin are also sold as nutritional supplements.^[citation needed]

Figure 1.4.1.6 The structure of inulin. Source: Wikipedia

As the name suggests, **polysaccharides** are substances built up by the condensation of a very large number of monosaccharide units. Cellulose, for example, is a polymer of β -glucose, containing upwards of 3000 glucose units in a chain. Starch is largely a polymer of α -glucose.

These two substances are a classic example of how a minor difference in the monomer can lead to major differences in the macroscopic properties of the polymer. Good-quality cotton and paper are almost pure cellulose, and they give us a good idea of its properties. Cellulose forms strong but flexible fibers and does not dissolve in water. By contrast, starch has no mechanical strength at all, and some forms are water soluble. Part of the molecular structure of cellulose and starch are shown in Fig. 1.4.1.6

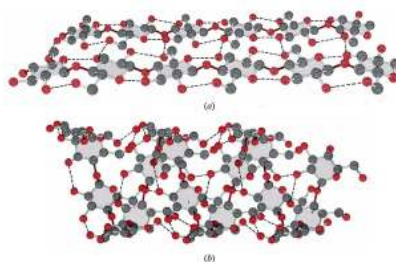


Figure 1.4.1.6 Structures of (a) cellulose and (b) amylose (starch). The C—O bonds linking glucose units are shown in color and hydrogen bonds are shown as single black lines. Hydrogen atoms have been omitted to simplify the structure. Note how the β -glucose units in cellulose form a linear chain because the C—O hands on either side of the glucose unit are parallel. In amylose, where α -glucose is the monomer, the chain is forced to curve. Note also the numerous hydrogen bonds between the two cellulose chains shown and the hydrogen bonds connecting successive turns of the spiral chain of amylose. When iodine contacts starch, I_2 molecules can fit lengthwise within the spiral of each amylose molecule. The starch-iodine complex which results is responsible for the dark blue color observed when iodine contacts starch.

Cellulose and starch are different not only in overall structure and macroscopic properties. From a biochemical point of view they behave so differently that it is difficult to believe that they are both polymers of the same monosaccharide. Enzymes which are capable of hydrolyzing starch will not touch cellulose, and vice versa. From a plant's point of view this is just as well since cellulose makes up structural material while starch serves as a storehouse for energy. If there were not a sharp biochemical distinction between the two, the need for a bit more energy by the plant might result in destruction of cell walls or other necessary structural components.

Starches in Food

Starch is the most common carbohydrate in the human diet and is contained in many staple foods. The major sources of starch intake worldwide are the cereals (rice, wheat, and maize) and the root vegetables (potatoes and cassava). Many other starchy foods are grown, some only in specific climates, including acorns, arrowroot, arracacha, bananas, barley, breadfruit, buckwheat, canna, colocasia, katakuri, kudzu, malanga, millet, oats, oca, polynesian arrowroot, sago, sorghum, sweet potatoes, rye, taro, chestnuts, water chestnuts and yams, and many kinds of beans, such as favas, lentils, mung beans, peas, and chickpeas.

Widely used prepared foods containing starch are bread, pancakes, cereals, noodles, pasta, porridge and tortilla.

Digestive enzymes have problems digesting crystalline structures. Raw starch is digested poorly in the duodenum and small intestine, while bacterial degradation takes place mainly in the colon. When starch is cooked, the digestibility is increased. Starch gelatinization during cake baking can be impaired by sugar competing for water, preventing gelatinization and improving texture.

Before the advent of processed foods, people consumed large amounts of uncooked and unprocessed starch-containing plants, which contained high amounts of resistant starch. Microbes within the large intestine fermented the starch, produced short-chain fatty acids, which are used as energy, and support the maintenance and growth of the microbes. More highly processed foods are more easily digested and release more glucose in the small intestine—less starch reaches the large intestine and more energy is absorbed by the body. It is thought that this shift in energy delivery (as a result of eating more processed foods) may be one of the contributing factors to the development of metabolic disorders of modern life, including obesity and diabetes.

Fibers in Food

Dietary fiber (British spelling **fibre**) or **roughage** is the portion of plant-derived food that cannot be completely broken down by human digestive enzymes. Dietary fiber consists of non-starch polysaccharides and other plant components such as cellulose, resistant starch, resistant dextrins, inulin, lignins, chitins, pectins, beta-glucans, and oligosaccharides.

Polysaccharide fiber differs from other polysaccharides in that it contains beta-glycosidic bonds (as opposed to alpha-glycosidic bonds). To illustrate these differences, consider the structural differences between amylose and cellulose (type of fiber) in the figure below. Both are linear chains of glucose, the only difference is that amylose has alpha-glycosidic bonds, while cellulose has beta-glycosidic bonds as shown below. The beta-bonds in fiber cannot be broken down by the digestive enzymes in the small intestine so they continue into the large intestine.

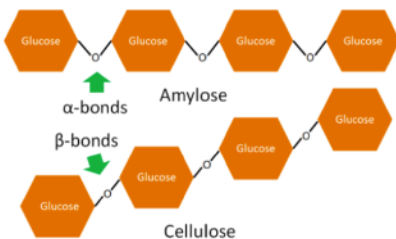


Figure 1.4.1.7 Structures of amylose and cellulose

Fiber can be classified by its physical properties. In the past, fibers were commonly referred to as soluble and insoluble. This classification distinguished whether the fiber was soluble in water. However, this classification is being phased out in the nutrition community. Instead, most fibers that would have been classified as insoluble fiber are now referred to as **nonfermentable and/or nonviscous** and **soluble fiber as fermentable, and/or viscous** because these better describe the fiber's characteristics. **Viscous** refers to the capacity of certain fibers to form a thick gel-like consistency.

Fermentable (soluble fiber) dissolves in water and is readily fermented in the colon into gases and physiologically active by-products, such as short-chain fatty acids produced in the colon by gut bacteria; it is viscous, may be called prebiotic fiber, and delays gastric emptying which, in humans, can result in an extended feeling of fullness.

Non-fermentable (insoluble fiber) does not dissolve in water and is inert to digestive enzymes in the upper gastrointestinal tract and provides bulking. Some forms of insoluble fiber, such as resistant starches, can be fermented in the colon. Bulking fibers absorb water as they move through the digestive system, easing defecation.

Table 1.4.1.4 lists some of the common types of fiber and provides a brief description about each. Specific sources of the different types of soluble and insoluble fiber as well as the amount of fiber found in common foods are discussed in section 17.4.

Table 1.4.1.4 Common Types of Fermentable (Soluble) Fiber and Non-Fermentable (Insoluble) Fiber.

Fermentable (Soluble) Fiber	Description	Non-Fermentable (Insoluble Fiber)	Description
Hemicellulose (soluble type)	Surround cellulose in plant cell walls	Cellulose	Main component of plant cell walls
Pectin	Found in cell walls and intracellular tissues of fruits and berries	Hemicellulose (insoluble type)	Surround cellulose in plant cell walls
Beta-glucans	Found in cereal brans	Lignin	Non carbohydrate found within "woody" plant cell walls
Gums	Viscous, usually isolated from seeds		

Summary

- Carbohydrate digestion begins in the mouth (in the presence of salivary α -amylase) and continues in the small intestine. The major products of the complete hydrolysis of disaccharides and polysaccharides are three monosaccharide units: glucose, fructose, and galactose. These are absorbed through the wall of the small intestine into the bloodstream.
- Simple sugars like glucose, fructose and the disaccharide sucrose function as natural sweeteners.
- More complex carbohydrates (oligosaccharides and polysaccharides) are now significant parts of the daily diet promoting gut health that leads to other health benefits.

Contributors and Attributions

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- Libretext: Basics of GOB Chemistry (Ball, et al.)
- [Template:ContribLindshield](#)
-
- Wikipedia
- US FDA
- [Marisa Alviar-Agnew](#) ([Sacramento City College](#))

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1.4.2: Fats and Cholesterol

Learning Objectives

- Describe the digestion of lipids.
- Know the properties and functions of the different types of lipoproteins.
- Know the sources and function of common dietary lipids.

How Does Fat Differ From Lipids? The answer you receive from this question will depend on who you ask, so it is important to have an understanding of lipids and fats from a chemical and nutritional perspective.

To a chemist, lipids consist of triglycerides, fatty acids, phospholipids, waxes, and sterols. These compounds are grouped together because of their structural and physical property similarities. For instance, all lipids have hydrophobic (water-fearing) properties. Chemists further separate lipids into fats and oils based on their physical properties at room temperature:

- **Fats** are solid at room temperature
- **Oils** are liquid at room temperature

From a nutritional perspective, the definition of lipids is the same. The definition of a fat differs, however, because nutrition-oriented people define fats based on their caloric contribution rather than whether they are solid at room temperature. Thus, from a nutrition perspective, **Fats** are triglycerides, fatty acids, and phospholipids that provide 9 kcal/g. The other difference is that from a caloric perspective, an oil is a fat. For example, let's consider olive oil. Clearly, it is an oil according to a chemist definition, but from a caloric standpoint it is a fat because it provides 9 kcal/g.

Digestion of Lipids

Lipid digestion begins in the upper portion of the small intestine (Figure 1.4.2.1). A hormone secreted in this region stimulates the gallbladder to discharge bile into the duodenum. The principal constituents of bile are the bile salts, which emulsify large, water-insoluble lipid droplets, disrupting some of the hydrophobic interactions holding the lipid molecules together and suspending the resulting smaller globules (micelles) in the aqueous digestive medium. These changes greatly increase the surface area of the lipid particles, allowing for more intimate contact with the lipases and thus rapid digestion of the fats. Another hormone promotes the secretion of pancreatic juice, which contains these enzymes.

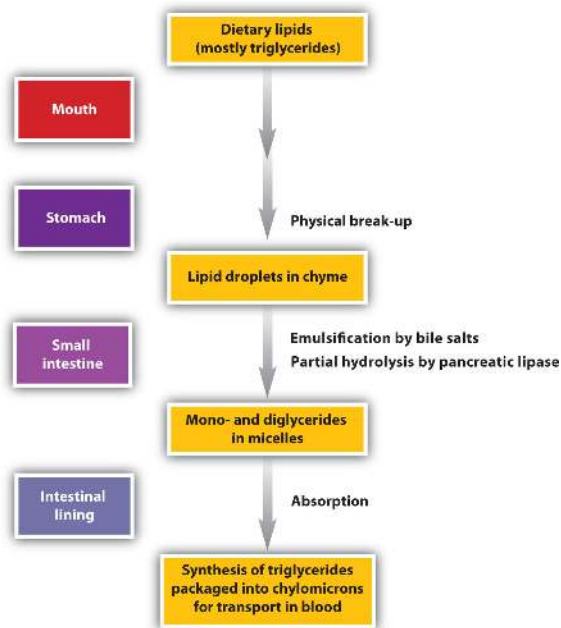
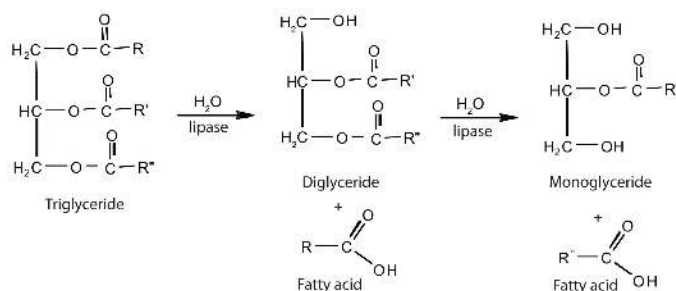


Figure 1.4.2.1 The principal events and sites of lipid (primarily triglyceride) digestion.

The lipases in pancreatic juice catalyze the digestion of triglycerides first to diglycerides and then to 2-monoglycerides and fatty acids:



The monoglycerides and fatty acids cross the intestinal lining into the bloodstream, where they are resynthesized into triglycerides and transported as lipoprotein complexes known as chylomicrons. Phospholipids and cholesteryl esters undergo similar hydrolysis in the small intestine, and their component molecules are also absorbed through the intestinal lining.

Fats, Cholesterol, and Human Health

The primary sterol that we consume is **cholesterol**. The structure of cholesterol is shown below.

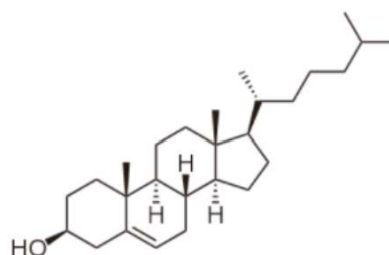


Figure 1.4.2.2 The carbon ring structure of cholesterol¹

Cholesterol is frequently found in foods as a cholesterol ester, meaning that there is a fatty acid attached to it. The structure of a cholesterol ester is shown below. All sterols have a similar structure to cholesterol. Cholesterol is only found in foods of animal origin. If consumers were more knowledgeable, intentionally misleading practices, such as labeling a banana “cholesterol free”, would not be as widespread as they currently are today.

Function

Although cholesterol has acquired the status of a nutrition “villain”, it is a vital component of cell membranes and is used to produce vitamin D, hormones, and bile acids. You can see the similarity between the structures of vitamin D and estradiol, one of the forms of estrogen shown below.



Figure 1.4.2.3 Structures of vitamin D₃ and estradiol (a form of estrogen)^{2,3}

We do not need to consume any cholesterol from our diets (not essential) because our bodies have the ability to synthesize the required amounts. The figure below gives you an idea of the cholesterol content of a variety of foods.

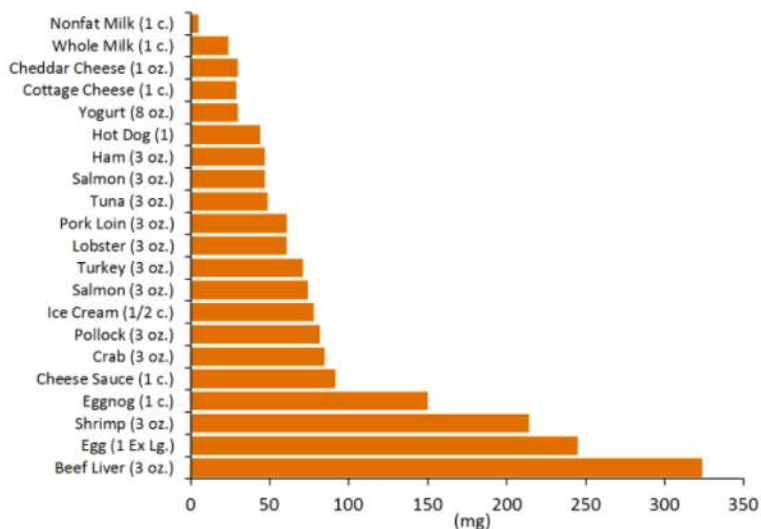


Figure 1.4.2.4 The cholesterol content (mg) of foods⁴

There is neither bad nor good cholesterol, despite these descriptions being commonly used for LDL and HDL, respectively. Cholesterol is cholesterol. HDL and LDL contain cholesterol but are actually lipoproteins that will be described below.

Too much cholesterol in the blood can combine with other substances to form plaque. Plaque sticks to the walls of the arteries. This buildup of plaque is known as [atherosclerosis](#). It can lead to [coronary artery disease](#), wherein the coronary arteries become narrow or even blocked.

The most common cause of high cholesterol is an unhealthy lifestyle. This can include:

- **Unhealthy eating habits**, such as eating lots of bad fats. One type, saturated fat, is found in some meats, dairy products, chocolate, baked goods, and deep-fried and processed foods. Another type, trans fat, is in some fried and processed foods. Eating these fats can raise your LDL (bad) cholesterol.
- **Lack of physical activity**, with lots of sitting and little exercise. This lowers your HDL (good) cholesterol.
- **Smoking**, which lowers HDL cholesterol, especially in women. It also raises your LDL cholesterol.

Genetics may also cause people to have high cholesterol. For example, familial hypercholesterolemia (FH) is an inherited form of high cholesterol. Other medical conditions and certain medicines may also cause high cholesterol.

HDL, LDL, and VLDL

Lipoproteins, as the name suggests, are complexes of lipids and protein. The proteins within a lipoprotein are called apolipoproteins (aka apoproteins). T

There are a number of lipoproteins in the body. They differ by the **apolipoproteins** they contain, size (diameter), density, and composition. The table below shows the difference in density and diameter of different lipoproteins. Notice that as diameter decreases, density increases.

Table \PageIndex{1} Properties of different lipoproteins.

Lipoprotein	Density (g/dL)	Diameter (nm)	Purpose
HDL (high-density lipoproteins)	1.063-1.21	5-12	It is sometimes called "good" cholesterol because it carries cholesterol from other parts of your body back to your liver. Your liver then removes the cholesterol from your body.
LDL (low-density lipoproteins)	1.019-1.063	18-25	It is sometimes called "bad" cholesterol because a high LDL level leads to the buildup of plaque in your arteries.

Lipoprotein	Density (g/dL)	Diameter (nm)	Purpose
VLDL (very low-density lipoproteins)	0.95-1.006	30-80	Some people also call VLDL a "bad" cholesterol because it too contributes to the buildup of plaque in your arteries. But VLDL and LDL are different; VLDL mainly carries triglycerides and LDL mainly carries cholesterol.

This inverse relationship is a result of the larger lipoproteins being composed of a higher percentage of triglyceride and a lower percentage of protein as shown below.

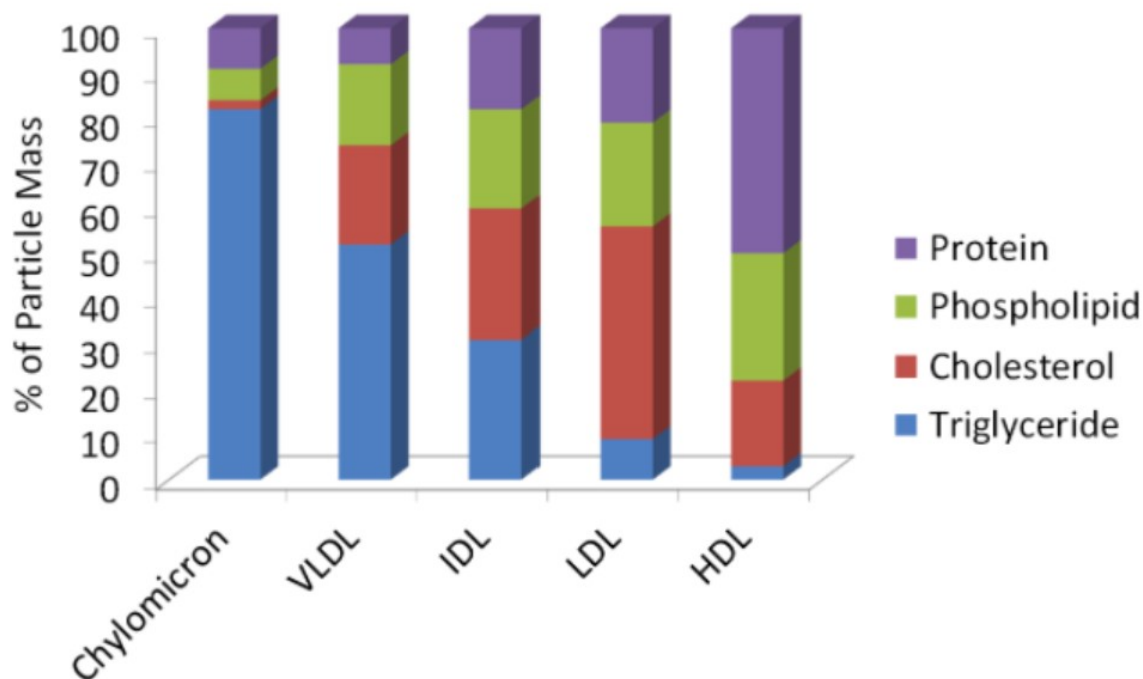


Figure 1.4.2.5 Composition of lipoproteins

Protein is more dense than triglyceride (why muscle weighs more than fat), thus the higher protein/lower triglyceride composition, the higher the density of the lipoprotein. Many of the lipoproteins are named based on their densities (i.e. very low-density lipoproteins).

You are probably familiar with HDL and LDL being referred to as "good cholesterol" and "bad cholesterol," respectively. This is an oversimplification to help the public interpret their blood lipid values, because cholesterol is cholesterol; it's not good or bad. LDL and HDL are lipoproteins, and as a result you can't consume good or bad cholesterol, you consume cholesterol. A more appropriate descriptor for these lipoproteins would be HDL "good cholesterol transporter" and LDL "bad cholesterol transporter."

What's so bad about LDL? LDL enters the endothelium where it is oxidized. This oxidized LDL is engulfed by white blood cells (macrophages), leading to the formation of what are known as foam cells. The foam cells eventually accumulate so much LDL that they die and accumulate, forming a fatty streak. From there the fatty streak, which is the beginning stages of a lesion, can continue to grow until it blocks the artery. This can result in a myocardial infarction (heart attack) or a stroke. HDL is good in that it scavenges cholesterol from other lipoproteins or cells and returns it to the liver. The figure below shows the formation of the fatty streak and how this can progress to a point where it greatly alters blood flow.

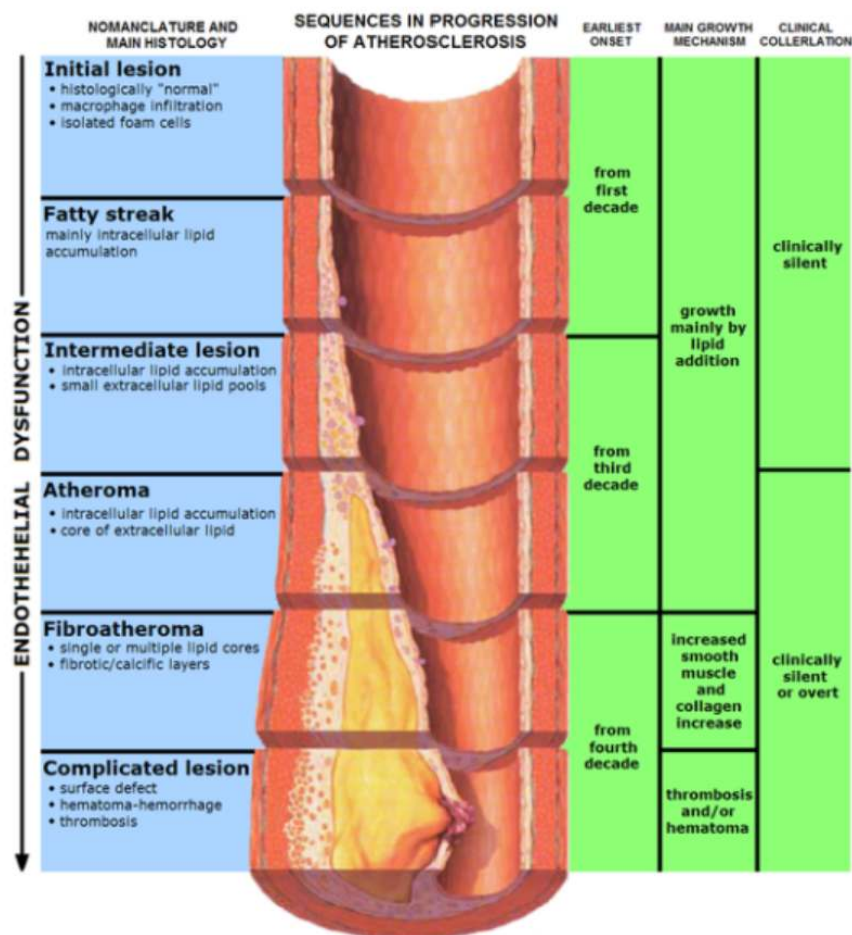


Figure 1.4.2.6 The formation of a lesion in an artery⁵

Web links

The video below does an excellent job of illustrating this process. However, there are two caveats to point out. First, it incorrectly refers to cholesterol (LDL-C etc.), and second, it is clearly made by a drug company, so keep these factors in mind. The link below is the American Heart Association's simple animation of how atherosclerosis develops.

[Video: Atherosclerosis \(5:36\)](#)

Cholesterol and CAD

Despite what you learned above about HDL, a recent study questions its importance in preventing cardiovascular disease. It found that people who have genetic variations that lead to higher HDL levels were not at decreased risk of developing cardiovascular disease. You can read more about this interesting finding in the first link below. In addition, another recent study is questioning whether saturated fat is associated with an increased risk of cardiovascular disease.

[Doubt Cast on the 'Good' in 'Good Cholesterol'](#)

[Study Questions Fat and Heart Disease Link](#)

The following video gives a general overview of macronutrient digestion, uptake, and absorption.

[Video: Small Intestine \(1:29\)](#)

[Saturated Fats, Unsaturated Fats, Essential Fatty Acids, and Trans Fats](#)

Chain Length of Fatty Acids

Fatty acids have different chain lengths, typically between four and 24 carbons, and most contain an even number of carbon atoms. When the carbon chain length is shorter, the melting point of the fatty acid becomes lower (such as fats found in dairy products) and the fatty acid becomes more liquid. Longer chain lengths tend to result in more solid fats, although melting point is also influenced by the degree of saturation.

Degrees of Saturation of Fatty Acids

Fatty acid chains are composed primarily of carbon and hydrogen atoms that are bonded to each other. The term “saturation” refers to whether the carbon atom in a fatty acid chain is filled (or “saturated”) to capacity with hydrogen atoms. In a **saturated fatty acid**, each carbon is bonded to two hydrogen atoms, with single bonds between the carbons.

Alternatively, fatty acids can have points where hydrogen atoms are missing, because there is a double bond between carbons ($C=C$). This is referred to as a point of unsaturation, because the carbon is only bonded to one hydrogen atom instead of two. **Unsaturated fatty acids** have one or more points of unsaturation, or double bonds between the carbons. A **monounsaturated fatty acid** is a fatty acid with one double bond, and a **polyunsaturated fatty acid** is a fatty acid with two or more double bonds.

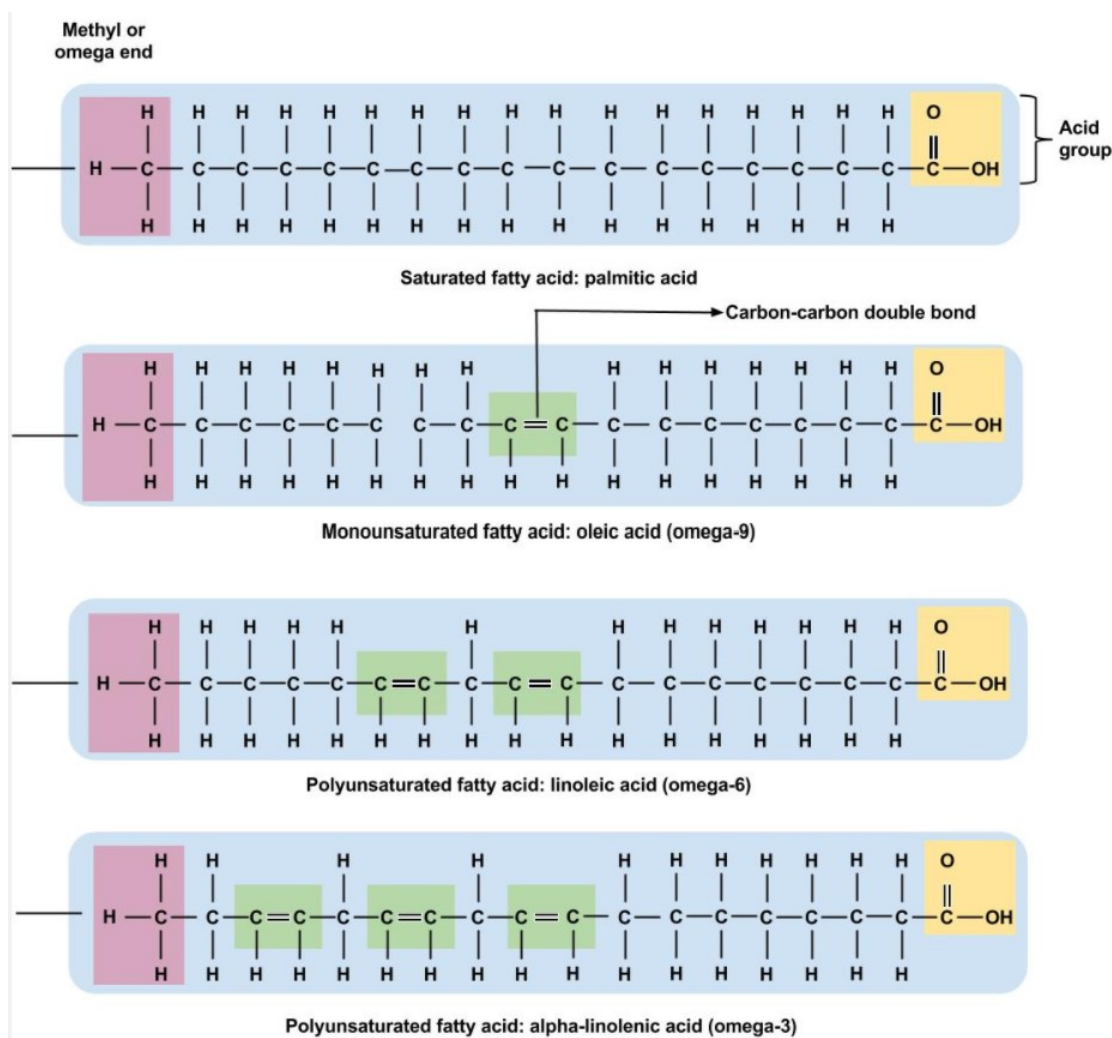


Figure 1.4.2.1: The structures of a saturated, monounsaturated, and polyunsaturated fat. Note the differences in points of unsaturation ($C=C$ double bonds) on some of the fatty acids.

Triglycerides in food contain a mixture of saturated, monounsaturated, and polyunsaturated fatty acids, but some foods are better sources of these types of fatty acids than others (Figure 5.13). For example, coconut oil is very high in saturated fat, but it still contains some monounsaturated and polyunsaturated fatty acids. Peanut oil is often thought of as a good source of

monounsaturated fat, because that is the predominant fatty acid in the oil, but peanut oil also contains a fair amount of polyunsaturated fatty acids and even some saturated fatty acids.

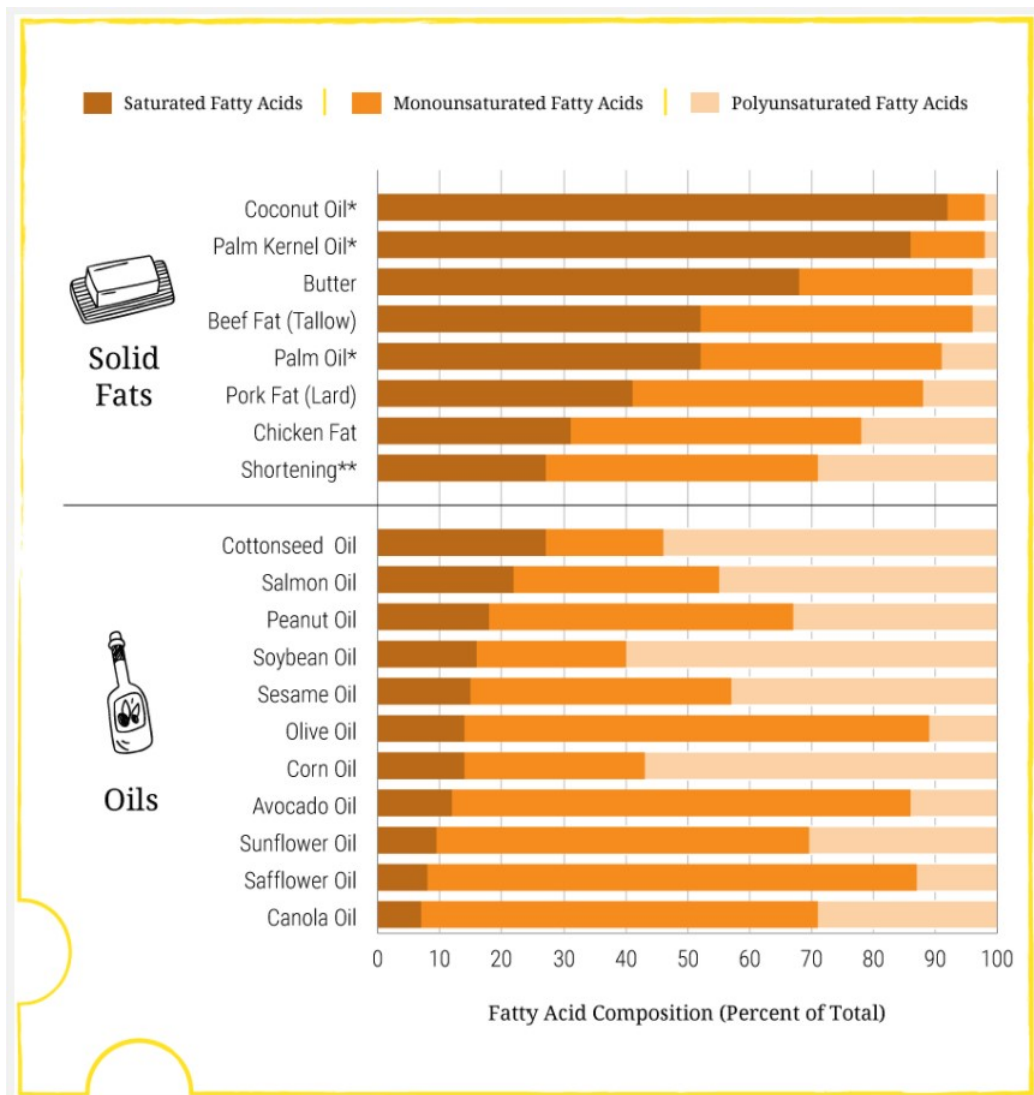


Figure 1.4.2.2: Dietary fats contain a mixture of saturated, monounsaturated, and polyunsaturated fatty acids. Foods are often categorized by the predominant type of fatty acids they contain, even though foods contain all three types. (Copyright; author via source)

Saturated Fatty Acids

Fat sources with a high percentage of **saturated fatty acids tend to be solid at room temperature**. This is because the lack of double bonds in the carbon chains of saturated fatty acids makes them very straight, so they pack together well (like a box of toothpicks). Fats that have mostly saturated fatty acids, like butter and coconut oil, are solid at room temperature, as are the visible fat layers in a strip of bacon or a cut of beef. Consuming a diet high in saturated fats is associated with an increased risk of heart disease, because such a diet increases blood cholesterol, specifically the LDL (“bad”) cholesterol level. (More on this later.) **Food sources of predominately saturated fatty acids** include most animal fats (with the exception of poultry and eggs, which contain more unsaturated fatty acids), dairy products, tropical oils (like coconut and palm oil), cocoa butter, and partially or fully hydrogenated oils.



Figure 1.4.2.3: Examples of foods high in saturated fat, such as meat and dairy products.

Unsaturated Fatty Acids

Fat sources rich in **unsaturated fatty acids** tend to be **liquid at room temperature**, because the $C=C$ double bonds create bends in the carbon chain, making it harder for fatty acids to pack together tightly. Consuming a diet rich in mono- and polyunsaturated fats is associated with a lower LDL cholesterol level and a lower risk of heart disease.

Food sources of predominately monounsaturated fats include nuts and seeds like almonds, pecans, cashews, and peanuts; plant oils like canola, olive, and peanut oils; and avocados. The fat in poultry and eggs is predominantly unsaturated and contains more monounsaturated than polyunsaturated fatty acids.

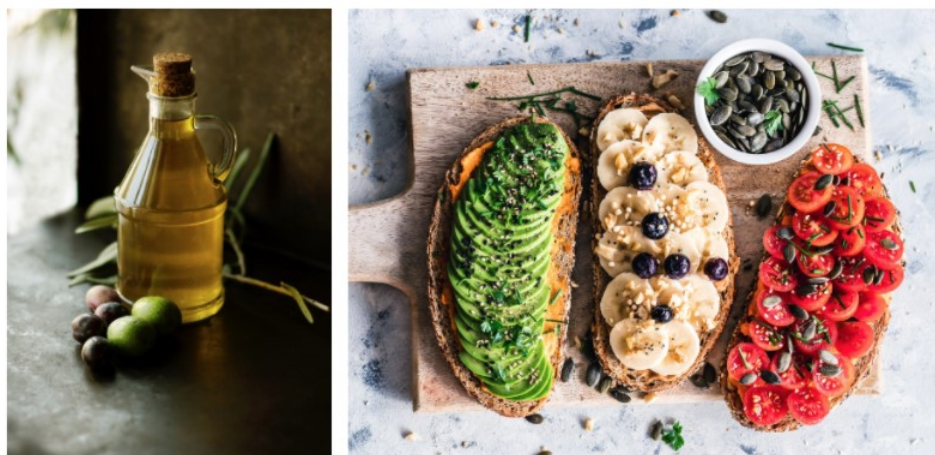


Figure 1.4.2.4: Examples of foods high in monounsaturated fat, such as olive oil, avocado, nut butters, and seeds. (Copyright; author via source).

Food sources of predominately polyunsaturated fats include plant oils (soybean, corn); fish; flaxseed; and some nuts like walnuts and pecans.

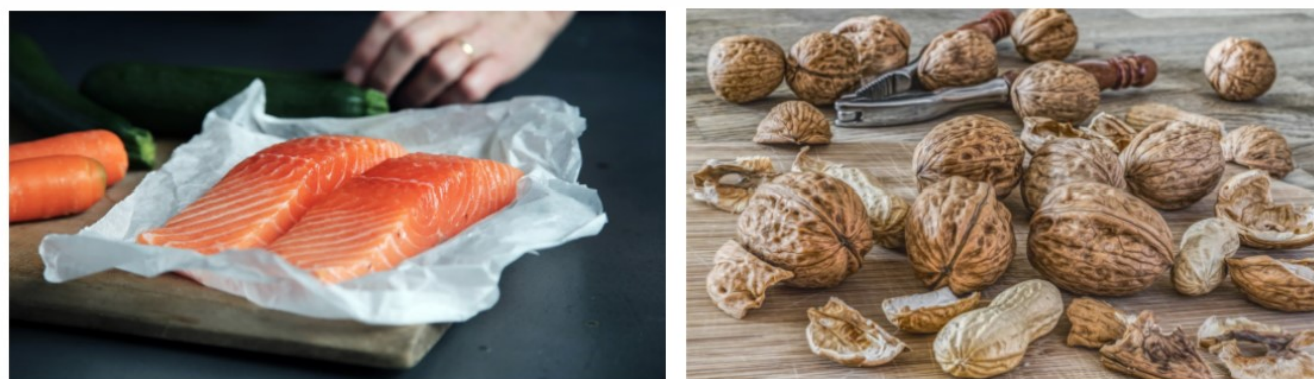


Figure 1.4.2.5: Examples of foods high in polyunsaturated fats, like fish and nuts.

Omega-3, Omega-6, and Essential Fatty Acids

In addition to the length of the carbon chain and the number of double bonds, **unsaturated fatty acids are also classified by the position of the first double bond relative to the methyl (-CH₃) or “omega” end of the carbon chain** (the end furthest from the glycerol backbone in a triglyceride). Fatty acids with the first double bond at the third carbon from the omega end are called **omega-3 fatty acids**. Those with the first double bond at the sixth carbon from the omega end are called **omega-6 fatty acids**. (There are also omega-9 fatty acids.)

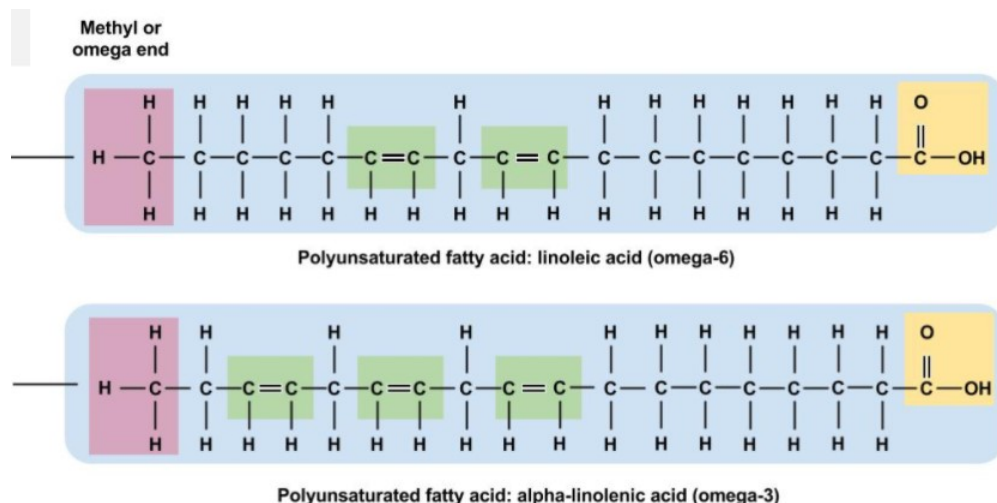
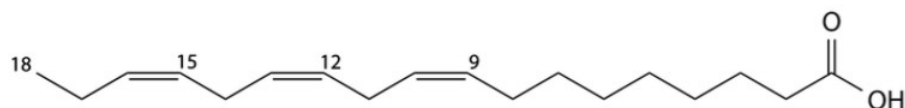
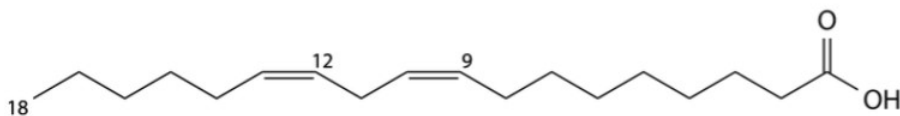


Figure 1.4.2.6: The position of the first C=C double bond determines whether an unsaturated fatty acid is classified as omega-3 or omega-6. The two essential fatty acids, linoleic acid (an omega-6) and alpha-linolenic acid (an omega-3) are shown here.

Fatty acids are vital for the normal operation of all body systems, but the body is capable of synthesizing most of the fatty acids it needs. However, there are two fatty acids that the body cannot synthesize: **linoleic acid** (an omega-6) and **alpha-linolenic acid** (ALA, an omega-3). These are called **essential fatty acids** because they must be consumed in the diet. Other fatty acids are called nonessential fatty acids, but that doesn't mean they're unimportant; the classification is based solely on the ability of the body to synthesize the fatty acid. Excellent **food sources of linoleic fatty acid** include plant oils such as corn oil and soybean oil, often found in salad dressings and margarine. **Rich food sources of alpha-linolenic acid (ALA)** include nuts, flaxseed, whole grains, legumes, and dark green leafy vegetables.



Alpha-linolenic acid (ALA). Note the first double bond occurs at the third carbon from the omega end of the fatty acid, thus making it an omega-3 fatty acid.



Linoleic acid. Note the first double bond occurs at the sixth carbon from the omega end of the fatty acid, thus making it an omega-6 fatty acid.

Figure 1.4.2.7: The chemical structure of the essential fatty acids shown in shorthand, without individual carbon and hydrogen atoms marked.

Most Americans easily consume enough linoleic acid and other omega-6 fatty acids, because corn and soybean oil are common ingredients in our food supply. However, sources of ALA and other omega-3 fatty acids are less common in the American diet, and

many people could benefit from incorporating more sources of these into their diet. As an added benefit, whole foods rich in ALA come packaged with other healthful nutrients, like fiber, protein, vitamins, minerals, and phytochemicals.

A true **essential fatty acid deficiency** is rare in the developed world, but it can occur, usually in people who eat very low-fat diets or have impaired fat absorption. Symptoms include dry and scaly skin, poor wound healing, increased vulnerability to infections, and impaired growth in infants and children.¹

Omega-3 and omega-6 fatty acids are precursors to a large family of important signaling molecules called **eicosanoids** (prostaglandins are one type of eicosanoid). Among the many functions of eicosanoids in the body, one of the most important is to regulate inflammation. Without these hormone-like molecules, the body would not be able to heal wounds or fight off infections each time a foreign germ presented itself. In addition to their role in the body's immune and inflammatory processes, eicosanoids also help to regulate circulation, respiration, and muscle movement.

Eicosanoids derived from omega-6 fatty acids tend to increase blood pressure, blood clotting, immune response, and inflammation. These are necessary functions, but they can be associated with disease when chronically elevated. In contrast, eicosanoids derived from omega-3 fatty acids tend to lower blood pressure, inflammation, and blood clotting, functions that can benefit heart health. Omega-3 and omega-6 fatty acids compete for the same enzymatic pathways in the formation of different eicosanoids, so increasing omega-3 fatty acids in the diet may have anti-inflammatory effects.

Two additional omega-3 fatty acids with important health benefits are **eicosapentaenoic acid (EPA)** and **docosahexaenoic acid (DHA)**. These long-chain polyunsaturated fatty acids have been shown to help lower blood triglycerides and blood pressure, reduce inflammation, and prevent blood clot formation. They also promote normal growth and development in infants, especially in the development of the brain and eyes. Both of these important omega-3 fatty acids can be synthesized in the body from ALA, so **they are not considered essential fatty acids**. However, the rate of conversion of ALA to these omega-3s is limited, so it is beneficial to consume them regularly in the diet. **Fish, shellfish, fish oils, seaweed, and algae are all good sources of EPA and DHA.** DHA is also found in human breast milk in quantities dependent on the mother's own intake of DHA sources.

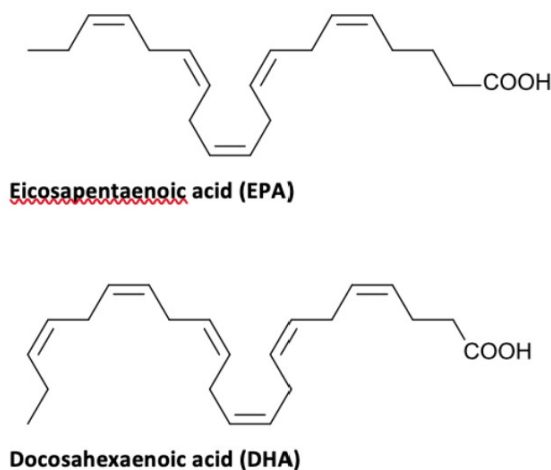


Figure 1.4.2.8: EPA and DHA are important but non-essential omega-3 fatty acids that can be made in the body from ALA.

Fish oil and omega-3 supplements are among the most commonly used dietary supplements in the United States. Researchers have hypothesized that these supplements might decrease risk of cardiovascular disease, be helpful for those with rheumatoid arthritis, and improve infant brain development when taken in pregnancy or in infancy. Some studies have found such benefits of the supplements, but others haven't. One reason for these inconsistent results may be that studies often don't measure participants' baseline omega-3 levels and intake from foods, and those already consuming adequate omega-3s are less likely to benefit from a supplement. The Dietary Guidelines for Americans recommends consuming 8 ounces of a variety of seafood each week, and in general, people who meet this recommendation likely consume enough omega-3 fatty acids already (along with the other healthful nutrients found in fish) and are unlikely to see an added benefit of taking a fish oil supplement. Some doctors may recommend that people at risk of cardiovascular disease take a fish oil or omega-3 supplement, especially if they don't eat fish regularly.²

A Word About *Trans* Fats

The carbon-carbon double bond in an unsaturated fatty acid chain can result in different shapes depending on whether the fatty acid is in a *cis* or *trans* configuration. When the hydrogen atoms are bonded to the same side of the carbon chain, it is called a *cis* fatty acid. Because the hydrogen atoms are on the same side (and repelling one another), the carbon chain has a bent structure. Naturally-occurring fatty acids usually have a *cis* configuration.

In a ***trans* fatty acid**, the hydrogen atoms are bonded on opposite sides of the carbon chain, resulting in a more linear structure. Unlike *cis* fatty acids, most *trans* fatty acids are not found naturally in foods, but instead are a result of an industrial process called hydrogenation. **Hydrogenation** is the process of adding hydrogen to the carbon-carbon double bonds, thus making the fatty acid saturated (or less unsaturated, in the case of partial hydrogenation).

Hydrogenation creates both saturated and trans fatty acids. Trans fatty acids are actually unsaturated fatty acids, but they have the linear shape of saturated fatty acids. (The carbon chains are not bent like naturally-occurring unsaturated fats.) **The trans fatty acids formed through partial hydrogenation have an unusual shape, which makes their properties and actions in the body similar to saturated fatty acids.**

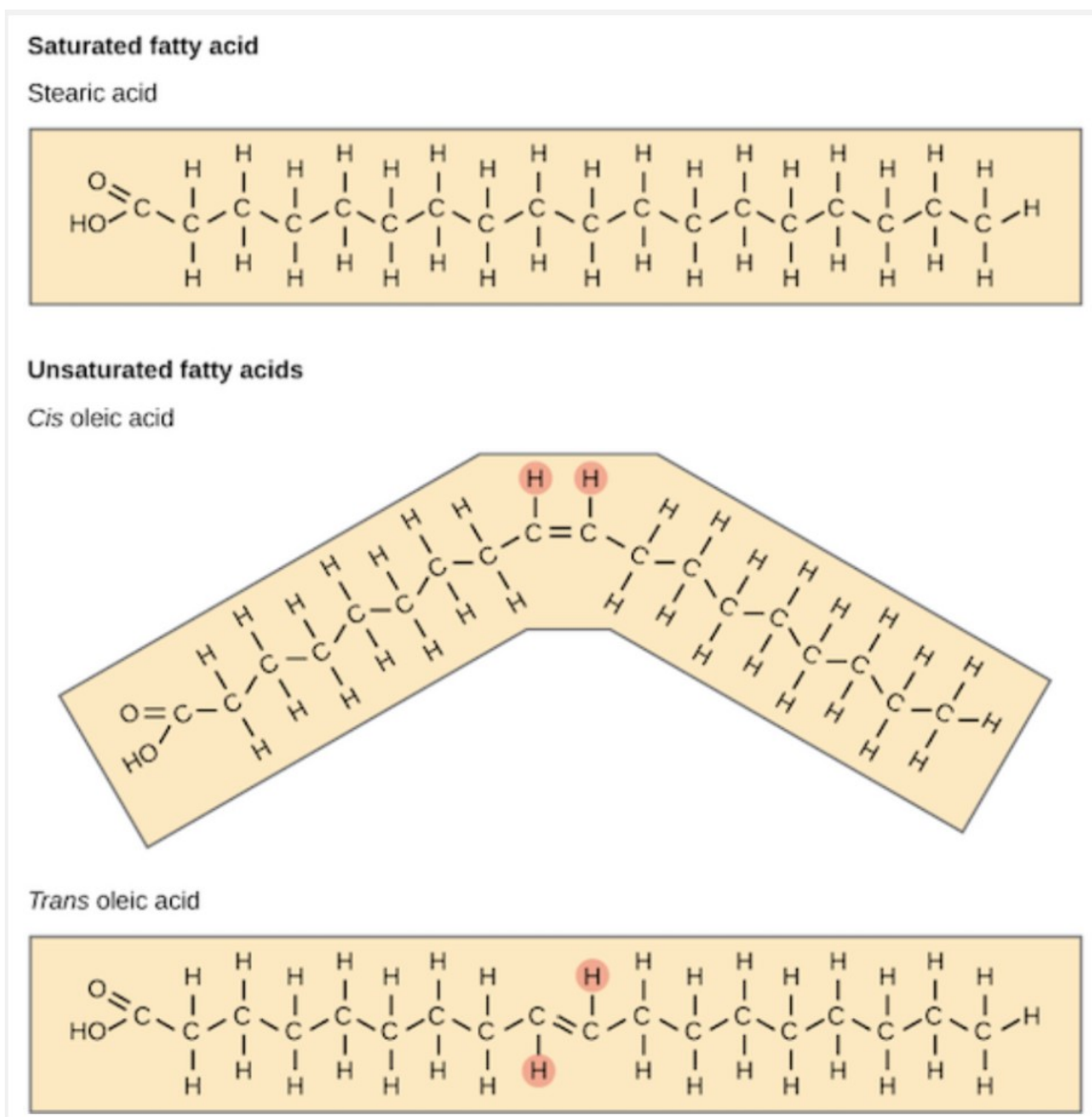


Figure 1.4.2.9: Comparison of a saturated fatty acid to both the *cis* and *trans* forms of an unsaturated fatty acid.

Hydrogenation was developed in order to make oils semi-solid at room temperature, enabling production of spreadable margarine and shortening from inexpensive ingredients like corn oil. Hydrogenation also makes oils more stable and less likely to go rancid,

so partially hydrogenated oils were favored by fast food restaurants for frying, and manufacturers of processed baked goods like cookies and chips found they gave their products a longer shelf life. And because trans fats are unsaturated, nutrition scientists and the medical community believed that they were a healthier alternative to saturated fats.

But around the 1990s, evidence that trans fats were not healthy—far worse than saturated fats, in fact—began to accumulate. Like saturated fat, **trans fats increase LDL (“bad”) cholesterol, but they also have the effect of decreasing HDL (“good”) cholesterol** and of increasing inflammatory processes in the body. Researchers found that consuming trans fats, even at low levels (1 to 3 percent of total energy intake), was associated with an increased risk of coronary heart disease. They estimated that eliminating industrial trans fats from the food supply might prevent as many as 19 percent of heart attacks in the U.S. at the time, coming to 228,000 heart attacks averted.³

In 2006, the U.S. Food and Drug Administration (FDA) began requiring food companies to list trans fat information on the Nutrition Facts panel of food labels to keep consumers informed of their intake of these fats. That prompted the food industry to mostly eliminate partially hydrogenated oils from their products, often substituting palm oil and coconut oil in their place (both of which are high in saturated fat and may promote heart disease). In 2013, the FDA determined that trans fats were no longer considered safe in the food supply, and in 2015, the agency issued a ruling requiring that manufactured trans fats no longer be included in the U.S. food supply. A one-year extension was granted in 2018, and foods produced prior to that date were given time to work through the food supply. The final ruling requires all manufactured trans fats to be eliminated from the U.S. food supply by 2021.⁴

Summary

- Digestion of lipids by lipases in pancreatic juice occurs primarily in the small intestines. The monoglycerides and fatty acids cross the intestinal lining into the bloodstream, where they are resynthesized into triglycerides and transported as chylomicrons. Phospholipids and cholesteryl esters undergo similar hydrolysis in the small intestine, and their component molecules are also absorbed through the intestinal lining.
- Two lipoproteins (composed of a lipid and a protein) of great interest are HDL "good cholesterol transporter" and LDL "bad cholesterol transporter."
- **Trans fats** are unhealthy fats that form when vegetable oil hardens in a process called hydrogenation. They can raise LDL cholesterol levels in the blood. They can also lower HDL (good) cholesterol levels. Trans fats are under review for their health effects.
- Saturated fats are also considered as unhealthy fats.
- Studies indicate that the consumption of monounsaturated fats and polyunsaturated fats (specifically those with omega-3 fatty acids) have numerous health benefits.

Contributors and Attributions

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1.4.3: Proteins- Muscle and Much More

Learning Objectives

- Describe the metabolism of proteins.
- Know the importance of essential amino acids.
- Know the sources and function of common proteins in the diet.

Proteins are essential nutrients for the human body. They are one of the building blocks of body tissue and can also serve as a fuel source. As a fuel, proteins provide as much energy density as carbohydrates: 4 kcal (17 kJ) per gram; in contrast, lipids provide 9 kcal (37 kJ) per gram. The most important aspect and defining characteristic of protein from a nutritional standpoint is its amino acid composition.

Proteins are polymer chains made of amino acids linked together by peptide bonds. During human digestion, proteins are broken down in the stomach to smaller polypeptide chains via hydrochloric acid and protease actions. This is crucial for the absorption of the essential amino acids that cannot be biosynthesized by the body.

Protein Functions in Human Body

Protein is a nutrient needed by the human body for growth and maintenance. Aside from water, proteins are the most abundant kind of molecules in the body. Protein can be found in all cells of the body and is the major structural component of all cells in the body, especially muscle. This also includes body organs, hair and skin. Proteins are also used in membranes, such as glycoproteins. When broken down into amino acids, they are used as precursors to nucleic acid, co-enzymes, hormones, immune response, cellular repair, and other molecules essential for life. Additionally, protein is needed to form blood cells.

Protein Metabolism: Essential Amino Acids

Protein digestion begins in the stomach (Figure 1.4.3.3), where the action of gastric juice hydrolyzes about 10% of the peptide bonds. Gastric juice is a mixture of water (more than 99%), inorganic ions, hydrochloric acid, and various enzymes and other proteins.

The pain of a gastric ulcer is at least partially due to irritation of the ulcerated tissue by acidic gastric juice.

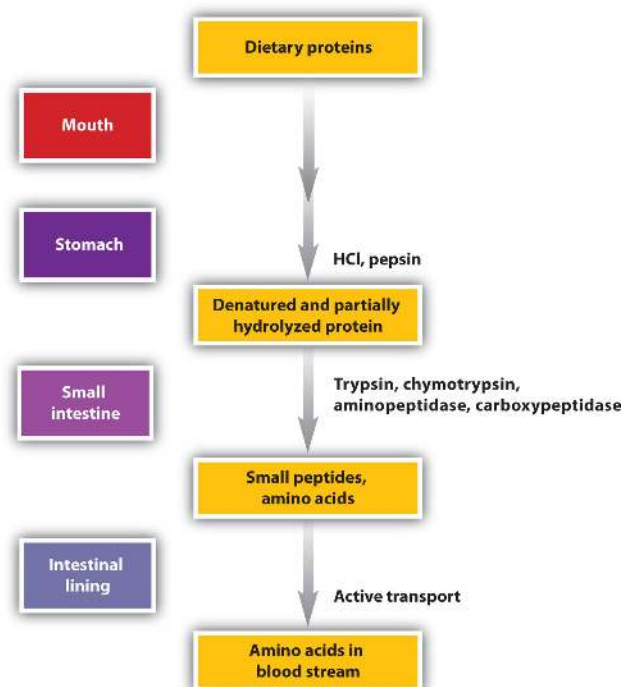


Figure 1.4.3.1 The principal events and Sites of Protein Digestion

The hydrochloric acid (HCl) in gastric juice is secreted by glands in the stomach lining. The pH of freshly secreted gastric juice is about 1.0, but the contents of the stomach may raise the pH to between 1.5 and 2.5. HCl helps to denature food proteins; that is, it unfolds the protein molecules to expose their chains to more efficient enzyme action. The principal digestive component of gastric juice is pepsinogen, an inactive enzyme produced in cells located in the stomach wall. When food enters the stomach after a period of fasting, pepsinogen is converted to its active form—pepsin—in a series of steps initiated by the drop in pH. Pepsin catalyzes the hydrolysis of peptide linkages within protein molecules. It has a fairly broad specificity but acts preferentially on linkages involving the aromatic amino acids tryptophan, tyrosine, and phenylalanine, as well as methionine and leucine.

Protein digestion is completed in the small intestine.

Amino Acids

There are 20 amino acids our body uses to synthesize proteins. These amino acids can be classified as essential, non-essential, or conditionally essential. The table below shows how the 20 amino acids are classified.

Table 1.4.3.1: Essential, conditionally essential, and nonessential amino acids

Essential	Conditionally Essential	Non-essential
Histidine	Arginine	Alanine
Isoleucine	Cysteine	Asparagine
Leucine	Glutamine	Aspartic Acid or Aspartate
Lysine	Glycine	Glutamic Acid or Glutamate
Methionine	Proline	Serine
Phenylalanine	Tyrosone	
Theronine		
Tryptophan		
Valine		

The body cannot synthesize nine amino acids. Thus, it is essential that these are consumed in the diet. As a result these amino acids are known as essential, or indispensable, amino acids.

Non-essential, or dispensable, amino acids can be made in our body, so we do not need to consume them. Conditionally essential amino acids become essential for individuals in certain situations. An example of a condition when an amino acid becomes essential is the disease *phenylketonuria (PKU)*. Individuals with PKU have a mutation in the enzyme phenylalanine hydroxylase, which normally adds an alcohol group (OH) to the amino acid phenylalanine to form tyrosine as shown below.

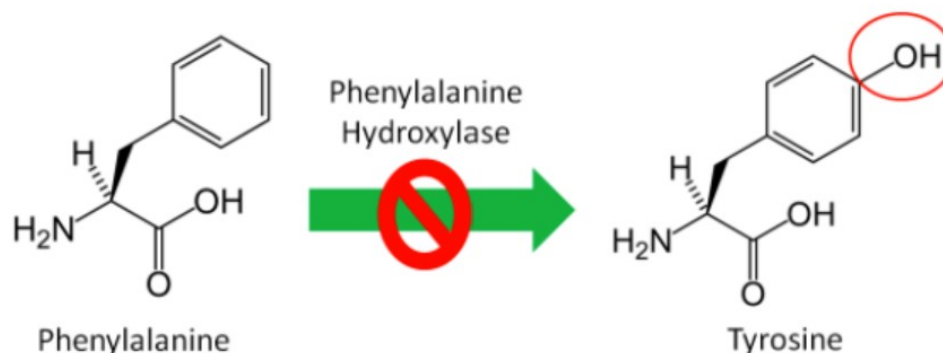


Figure 1.4.3.2: Phenylketonuria (PKU) results from a mutation in the enzyme phenylalanine hydroxylase

Since tyrosine cannot be synthesized by people with PKU, it becomes essential for them. Thus, tyrosine is a conditionally essential amino acid. Individuals with PKU have to eat a very low protein diet and avoid the alternative sweetener aspartame, because it can be broken down to phenylalanine. If individuals with PKU consume too much phenylalanine, phenylalanine and its metabolites, can build up and cause brain damage and severe mental retardation. The drug Kuvan was approved for use with PKU patients in 2007 who have low phenylalanine hydroxylase activity levels.

Protein Sources

Protein occurs in a wide range of food. On a worldwide basis, plant protein foods contribute over 60% of the per capita supply of protein. In North America, animal-derived foods contribute about 70% of protein sources. Insects are a source of protein in many parts of the world. In parts of Africa, up to 50% of dietary protein derives from insects. It is estimated that more than 2 billion people eat insects daily.

Meat, dairy, eggs, soy, fish, whole grains, and cereals are sources of protein. Examples of food staples and cereal sources of protein, each with a concentration greater than 7%, are (in no particular order) buckwheat, oats, rye, millet, maize (corn), rice, wheat, sorghum, amaranth, and quinoa. Some research highlights game meat as a protein source.

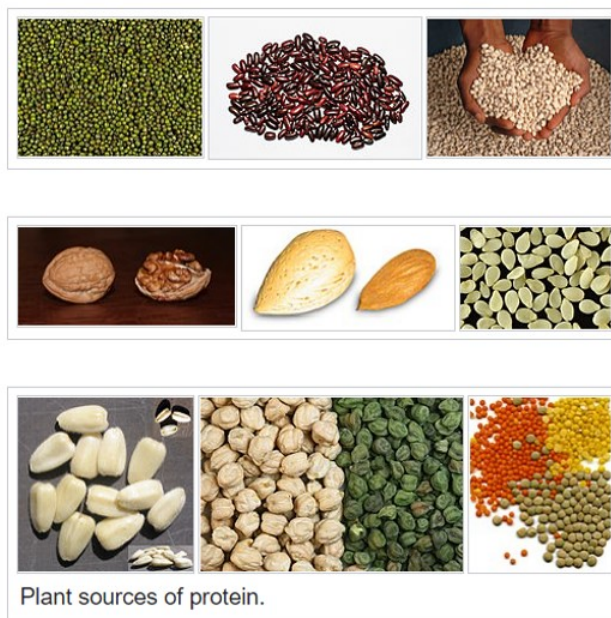


Figure 1.4.3.3 Typical sources of protein.

Vegan sources of proteins include legumes, nuts, seeds and fruits. Vegan foods with protein concentrations greater than 7% include soybeans, lentils, kidney beans, white beans, mung beans, chickpeas, cowpeas, lima beans, pigeon peas, lupines, wing beans, almonds, Brazil nuts, cashews, pecans, walnuts, cotton seeds, pumpkin seeds, hemp seeds, sesame seeds, and sunflower seeds.

People eating a balanced diet do not need protein supplements.

The table below presents food groups as protein sources.

Table 1.4.3.2 Density of amino acid in various protein sources.

Food source	Lysine	Threonine	Tryptophan	Sulfur-containing amino acids
Legumes	64	38	12	25
Cereals and whole grains	31	32	12	37
Nuts and seeds	45	36	17	46
Fruits	45	29	11	27
Animal	85	44	12	38

Colour key:

- Protein source with highest density of respective amino acid.
- Protein source with lowest density of respective amino acid.

Protein powders - such as casein, whey, egg, rice, soy, and cricket flour - are processed and manufactured sources of protein.

Complete and Incomplete Proteins

Proteins can be classified as either complete or incomplete. **Complete proteins** provide adequate amounts of all nine essential amino acids. Animal proteins such as meat, fish, milk, and eggs are good examples of complete proteins. **Incomplete proteins** do not contain adequate amounts of one or more of the essential amino acids. For example, if a protein doesn't provide enough of the essential amino acid leucine it would be considered incomplete. Leucine would be referred to as the limiting amino acid, because there is not enough of it for the protein to be complete. Most plant foods are incomplete proteins, with a few exceptions such as soy. The table below shows the limiting amino acids in some plant foods.

Table 1.4.3.3 Limiting amino acids in some common plant foods.

Food	Amino Acid(s)
Beans and Most Legumes	Methionine, Tryptophan
Tree Nuts and Seeds	Methionine, Lysine
Grains	Lysine
Vegetables	Methionine, Lysine

Complementary Proteins

Even though most plant foods do not contain complete proteins, it does not mean that they should be sworn off as protein sources. It is possible to pair foods containing incomplete proteins with different limiting amino acids to provide adequate amounts of the essential amino acids. These two proteins are called **complementary proteins**, because they supply the amino acid(s) missing in the other protein. A simple analogy would be that of a 4 piece puzzle. If one person has 2 pieces of a puzzle, and another person has 2 remaining pieces, neither of them have a complete puzzle. But when they are combined, the two individuals create a complete puzzle.



(Figure 1.4.3.4) Complementary proteins are kind of like puzzle pieces.

Two examples of complementary proteins are shown below.

Peanut Butter and Jelly Sandwich



Red Beans and Rice



Figure 1.4.3.5) Two complementary protein examples

It should be noted that complementary proteins do not need to be consumed at the same time or meal. It is currently recommended that essential amino acids be met on a daily basis, meaning that if a grain is consumed at one meal, a legume could be consumed at a later meal, and the proteins would still complement one another⁴.

Measures of Protein Quality

How do you know the quality of the protein in the foods you consume? The protein quality of most foods has been determined by one of the methods below.

- **Biological Value (BV)** - (grams of nitrogen retained / grams of nitrogen absorbed) x 100
- **Protein Efficiency Ratio (PER)** - (grams of weight gained / grams of protein consumed)

This method is commonly performed in growing rats.

- **Chemical or Amino Acid Score (AAS)** - (Test food limiting essential amino acid (mg/g protein) / needs of same essential amino acid (mg/g protein))
- **Protein Digestibility Corrected Amino Acid Score (PDCAAS)** - (Amino Acid Score x Digestibility)

This is the most widely used method and was preferred by the Food and Agriculture Organization and World Health Organization (WHO) until recently^{5,6}. The following table shows the protein quality measures for some common foods.

Table 1.4.3.4 Measures of protein quality

Protein	PER	Digestibility	AA(%)	PDCAAS
Egg	3.8	98	121	100*
Milk	3.1	95	127	100*
Beef	2.9	98	94	92

Protein	PER	Digestibility	AA(%)	PDCAAS
Soy	2.1	95	96	91
Wheat	1.5	91	47	42

*PDCAAS scores are truncated (cut off) at 100. These egg and milk scores are actually 118 and 121 respectively.

The Food and Agricultural Organization (FAO) recently recommended that PDCAAS be replaced with a new measure of protein quality, the Digestible Indispensable Amino Acid Score (DIAAS). "DIAAS is defined as: $\text{DIAAS \%} = 100 \times [(\text{mg of digestible dietary indispensable amino acid in 1 g of the dietary protein}) / (\text{mg of the same dietary indispensable amino acid in 1g of the reference protein})]$." Ileal digestibility should be utilized to determine the digestibility in DIAAS; ideally in humans, but if not possible in growing pigs or rats⁶.

The main differences between DIAAS and PDCAAS are:

1. DIAAS take into account individual amino acids digestibility rather than protein digestibility.
2. It focus on ileal instead of fecal (total) digestibility.
3. Has three different reference patterns (different age groups, 0-6 months, 6 months- 3 years, 3-10 years old) instead of a single pattern
4. DIAAS scores will not be truncated⁷

Protein Deficiency in Young and Old

Protein deficiency rarely occurs alone. Instead it is often coupled with insufficient energy intake. As a result, the condition is called protein-energy malnutrition (PEM). This condition is not common in the U.S., but is more prevalent in less developed countries. Kwashiorkor and marasmus are the two forms of protein energy malnutrition. They differ in the severity of energy deficiency as shown in the figure below.

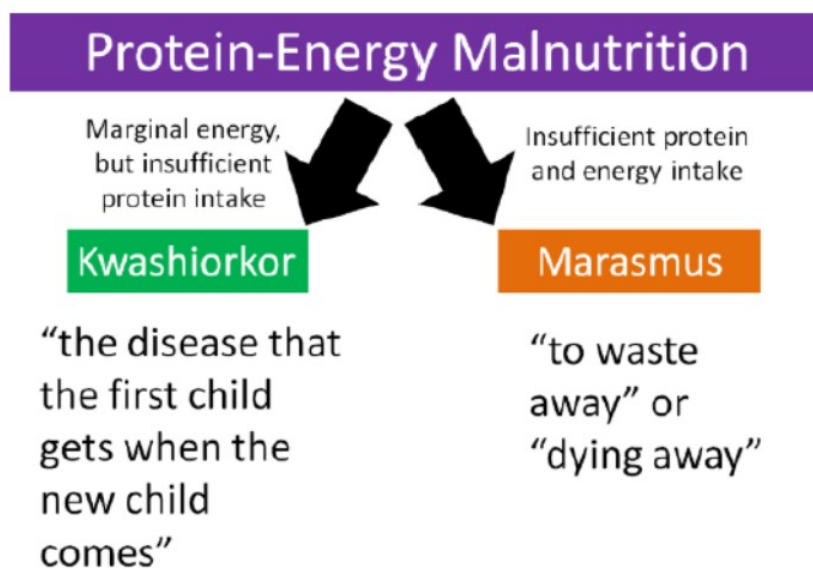


Figure 1.4.3.6 The two types of protein-energy malnutrition.

Kwashiorkor is a Ghanaian word that means "the disease that the first child gets when the new child comes³⁹." The characteristic symptom of kwashiorkor is a swollen abdomen. Energy intake could be adequate, but protein consumption is too low.



Figure 1.4.3.7: A child suffering from kwashiorkor

Marasmus means "to waste away" or "dying away", and thus occurs in individuals who have inadequate protein and energy intakes.



Figure 1.4.3.8 Two individuals suffering from marasmus

Summary

- Protein digestion begins in the stomach where hydrolysis of the protein linkages occurs with the action of gastric juices (mainly HCl) and the active enzyme pepsin. Protein digestion is completed in the small intestine wherein other protein digesting enzymes are involved.
- Essential amino acids cannot be made by the body and must come from food.
- Complete proteins provide adequate amounts of all nine essential amino acids.
- Complementary proteins are made up of two proteins wherein one protein supply the amino acid(s) missing in the other protein.
- Kwashiorkor and marasmus are two forms of protein energy malnutrition that are not common in the U.S., but is more prevalent in less developed countries

Contributors and Attributions

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1.4.4: Minerals, Vitamins, and Other Essentials

Learning Objectives

- List reasons why vitamins and minerals are critical to a healthy diet.
- Describe the functional role, intake recommendations and sources of vitamins and major minerals.
- Learn about the importance and sources of dietary fiber.
- Learn about the importance of water.

Vitamins and minerals are essential to human health and can be obtained in our diet from different types of food.

Dietary Minerals

Minerals in food are inorganic compounds that work with other nutrients to ensure the body functions properly. Minerals are abundant in our everyday lives. From the soil in your front yard to the jewelry you wear on your body, we interact with minerals constantly. There are 20 essential minerals that must be consumed in our diets to remain healthy. The amount of each mineral found in our bodies vary greatly and therefore, so does consumption of those minerals. When there is a deficiency in an essential mineral, health problems may arise.

Major minerals (Figure 1.4.4.1) are classified as minerals that are required in the diet each day in amounts larger than 100 milligrams. These include sodium, potassium, chloride, calcium, phosphorus, magnesium, and sulfur. These major minerals can be found in various foods. Consuming a varied diet significantly improves an individual's ability to meet their nutrient needs. The most common minerals in the body are calcium and phosphorous, both of which are stored in the skeleton and necessary for the hardening of bones. Most minerals are ionized, and their ionic forms are used in physiological processes throughout the body. Sodium and chloride ions are electrolytes in the blood and extracellular tissues, and iron ions are critical to the formation of hemoglobin. There are additional trace minerals that are still important to the body's functions, but their required quantities are much lower.

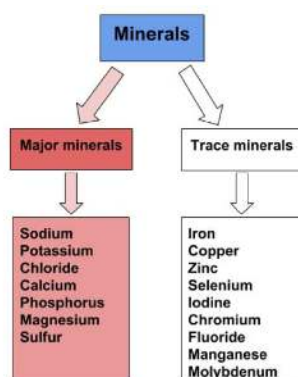


Figure 1.4.4.1 The major and trace minerals. Image by Allison Calabrese / CC BY 4.0.

Like vitamins, minerals can be consumed in toxic quantities (although it is rare). A healthy diet includes most of the minerals your body requires, so supplements and processed foods can add potentially toxic levels of minerals. Tables 1.4.4.1 and 1.4.4.2 provide a summary of minerals and their function in the body.

Table 1.4.4.1 Major Minerals and their Function in the Body.

Major Minerals				
Mineral	Sources	Recommended daily allowance	Function	Problems associated with deficiency

Major Minerals				
Mineral	Sources	Recommended daily allowance	Function	Problems associated with deficiency
Potassium	Meats, some fish, fruits, vegetables, legumes, dairy products	4700 mg	Nerve and muscle function; acts as an electrolyte	Hypokalemia: weakness, fatigue, muscle cramping, gastrointestinal problems, cardiac problems
Sodium	Table salt, milk, beets, celery, processed foods	2300 mg	Blood pressure, blood volume, muscle and nerve function	Rare
Calcium	Dairy products, dark green leafy vegetables, blackstrap molasses, nuts, brewer's yeast, some fish	1000 mg	Bone structure and health; nerve and muscle functions, especially cardiac function	Slow growth, weak and brittle bones
Phosphorous	Meat, milk	700 mg	Bone formation, metabolism, ATP production	Rare
Magnesium	Whole grains, nuts, leafy green vegetables	310–420 mg	Enzyme activation, production of energy, regulation of other nutrients	Agitation, anxiety, sleep problems, nausea and vomiting, abnormal heart rhythms, low blood pressure, muscular problems
Chloride	Most foods, salt, vegetables, especially seaweed, tomatoes, lettuce, celery, olives	2300 mg	Balance of body fluids, digestion	Loss of appetite, muscle cramps

Table 1.4.4.2 Trace Minerals and their Function in the Body.

Trace Minerals				
Mineral	Sources	Recommended daily allowance	Function	Problems associated with deficiency
Iron	Meat, poultry, fish, shellfish, legumes, nuts, seeds, whole grains, dark leafy green vegetables	8–18 mg	Transport of oxygen in blood, production of ATP	Anemia, weakness, fatigue
Zinc	Meat, fish, poultry, cheese, shellfish	8–11 mg	Immunity, reproduction, growth, blood clotting, insulin and thyroid function	Loss of appetite, poor growth, weight loss, skin problems, hair loss, vision problems, lack of taste or smell

Trace Minerals				
Mineral	Sources	Recommended daily allowance	Function	Problems associated with deficiency
Copper	Seafood, organ meats, nuts, legumes, chocolate, enriched breads and cereals, some fruits and vegetables	900 μg	Red blood cell production, nerve and immune system function, collagen formation, acts as an antioxidant	Anemia, low body temperature, bone fractures, low white blood cell concentration, irregular heartbeat, thyroid problems
Iodine	Fish, shellfish, garlic, lima beans, sesame seeds, soybeans, dark leafy green vegetables	150 μg	Thyroid function	Hypothyroidism: fatigue, weight gain, dry skin, temperature sensitivity
Sulfur	Eggs, meat, poultry, fish, legumes	None	Component of amino acids	Protein deficiency
Fluoride	Fluoridated water	3–4 mg	Maintenance of bone and tooth structure	Increased cavities, weak bones and teeth
Manganese	Nuts, seeds, whole grains, legumes	1.8–2.3 mg	Formation of connective tissue and bones, blood clotting, sex hormone development, metabolism, brain and nerve function	Infertility, bone malformation, weakness, seizures
Cobalt	Fish, nuts, leafy green vegetables, whole grains	None	Component of B ₁₂	None
Selenium	Brewer's yeast, wheat germ, liver, butter, fish, shellfish, whole grains	55 μg	Antioxidant, thyroid function, immune system function	Muscle pain
Chromium	Whole grains, lean meats, cheese, black pepper, thyme, brewer's yeast	25–35 μg	Insulin function	High blood sugar, triglyceride, and cholesterol levels
Molybdenum	Legumes, whole grains, nuts	45 μg	Cofactor for enzymes	Rare

The Vitamins: Vital, but Not All are Amines

In 1747, the Scottish surgeon James Lind discovered that citrus foods helped prevent scurvy, a particularly deadly disease in which collagen is not properly formed, causing poor wound healing, bleeding of the gums, severe pain, and death. In 1753, Lind published his *Treatise on the Scurvy*, which recommended using lemons and limes to avoid scurvy, which was adopted by the British Royal Navy. This led to the nickname *limey* for British sailors.

In East Asia, where polished white rice was the common staple food of the middle class, beriberi resulting from lack of vitamin B₁ was endemic. In 1884, Takaki Kanehiro, a British-trained medical doctor of the Imperial Japanese Navy, observed that beriberi was endemic among low-ranking crew who often ate nothing but rice, but not among officers who consumed a Western-style diet. This convinced Takaki and the Japanese Navy that diet was the cause of beriberi, but they mistakenly believed that sufficient amounts of protein prevented it. That diseases could result from some dietary deficiencies was further investigated by Christiaan Eijkman, who in 1897 discovered that feeding unpolished rice instead of the polished variety to chickens helped to prevent beriberi in the

chickens. The following year, Frederick Hopkins postulated that some foods contained "accessory factors" — in addition to proteins, carbohydrates, fats *etc.* — that are necessary for the functions of the human body. Hopkins and Eijkman were awarded the Nobel Prize for Physiology or Medicine in 1929 for their discoveries.

In 1910, the first vitamin complex was isolated by Japanese scientist Umetaro Suzuki, who succeeded in extracting a water-soluble complex of micronutrients from rice bran and named it aberic acid (later *Orizantin*). He published this discovery in a Japanese scientific journal. When the article was translated into German, the translation failed to state that it was a newly discovered nutrient, a claim made in the original Japanese article, and hence his discovery failed to gain publicity. In 1912 Polish-born biochemist Casimir Funk, working in London, isolated the same complex of micronutrients and proposed the complex be named "vitamine". It was later to be known as vitamin B₃ (niacin), though he described it as "anti-beri-beri-factor" (which would today be called thiamine or vitamin B₁). Funk proposed the hypothesis that other diseases, such as rickets, pellagra, coeliac disease, and scurvy could also be cured by vitamins.

Vitamine to Vitamin

Max Nierenstein a friend and reader of Biochemistry at Bristol University reportedly suggested the "vitamine" name (from "vital amine"). The name soon became synonymous with Hopkins' "accessory factors", and, by the time it was shown that not all vitamins are amines, the word was already ubiquitous. In 1920, Jack Cecil Drummond proposed that the final "e" be dropped to deemphasize the "amine" reference, after researchers began to suspect that not all "vitamines" (in particular, vitamin A) have an amine component.

LIX. THE NOMENCLATURE OF THE SO-CALLED ACCESSORY FOOD FACTORS (VITAMINS).

By JACK CECIL DRUMMOND.

From the Institute of Physiology, University College, London.

(Received August 12th, 1920.)

IN 1912 Hopkins published his classical paper in which he described the important influence of certain dietary constituents on the processes of growth and nutrition. These substances he termed the "accessory factors of the diet." At about the same time Funk, who was working on the subject of experimental beriberi, coined the name "Vitamine" for the same class of substances. Since then the literature has been a good deal confused by the great variety of names which have been utilised to denote these or similar dietary constituents (auximones, Bottomley; nutramines, Abderhalden, etc.). The criticism usually raised against Funk's word Vitamine is that the termination "-ine" is one strictly employed in chemical nomenclature to denote substances of a basic character, whereas there is no evidence which supports his original idea that these indispensable dietary constituents are amines. The word has, however, been widely adopted, and therefore until we know more about the actual nature of the substances themselves, it would be difficult and perhaps unwise to eliminate it altogether. The suggestion is now advanced that the final "-e" be dropped, so that the resulting word Vitamin is acceptable under the standard scheme of nomenclature adopted by the Chemical Society, which permits a neutral substance of undefined composition to bear a name ending in "-in." If this suggestion is adopted, it is recommended that the somewhat cumbrous nomenclature introduced by McCollum (Fat-soluble A, Water-soluble B), be dropped, and that the substances be spoken of as Vitamin A, B, C, etc. This simplified scheme should be quite sufficient until such time as the factors are isolated, and their true nature identified.

Figure 1.4.4.2 Jack Drummond's single-paragraph article in 1920 which provided structure and nomenclature used today for vitamins.

Vitamins are organic compounds found in foods and are a necessary part of the biochemical reactions in the body. They are involved in a number of processes, including mineral and bone metabolism, and cell and tissue growth, and they act as cofactors for energy metabolism. The B vitamins play the largest role of any vitamins in metabolism (Tables 1.4.4.3 and 1.4.4.4)

You get most of your vitamins through your diet, although some can be formed from the precursors absorbed during digestion. For example, the body synthesizes vitamin A from the β -carotene in orange vegetables like carrots and sweet potatoes. Vitamins are either fat-soluble or water-soluble. Fat-soluble vitamins A, D, E, and K, are absorbed through the intestinal tract with lipids in chylomicrons. Vitamin D is also synthesized in the skin through exposure to sunlight. Because they are carried in lipids, fat-soluble vitamins can accumulate in the lipids stored in the body. If excess vitamins are retained in the lipid stores in the body, hypervitaminosis can result.

Water-soluble vitamins, including the eight B vitamins and vitamin C, are absorbed with water in the gastrointestinal tract. These vitamins move easily through bodily fluids, which are water based, so they are not stored in the body. Excess water-soluble vitamins are excreted in the urine. Therefore, hypervitaminosis of water-soluble vitamins rarely occurs, except with an excess of vitamin supplements.

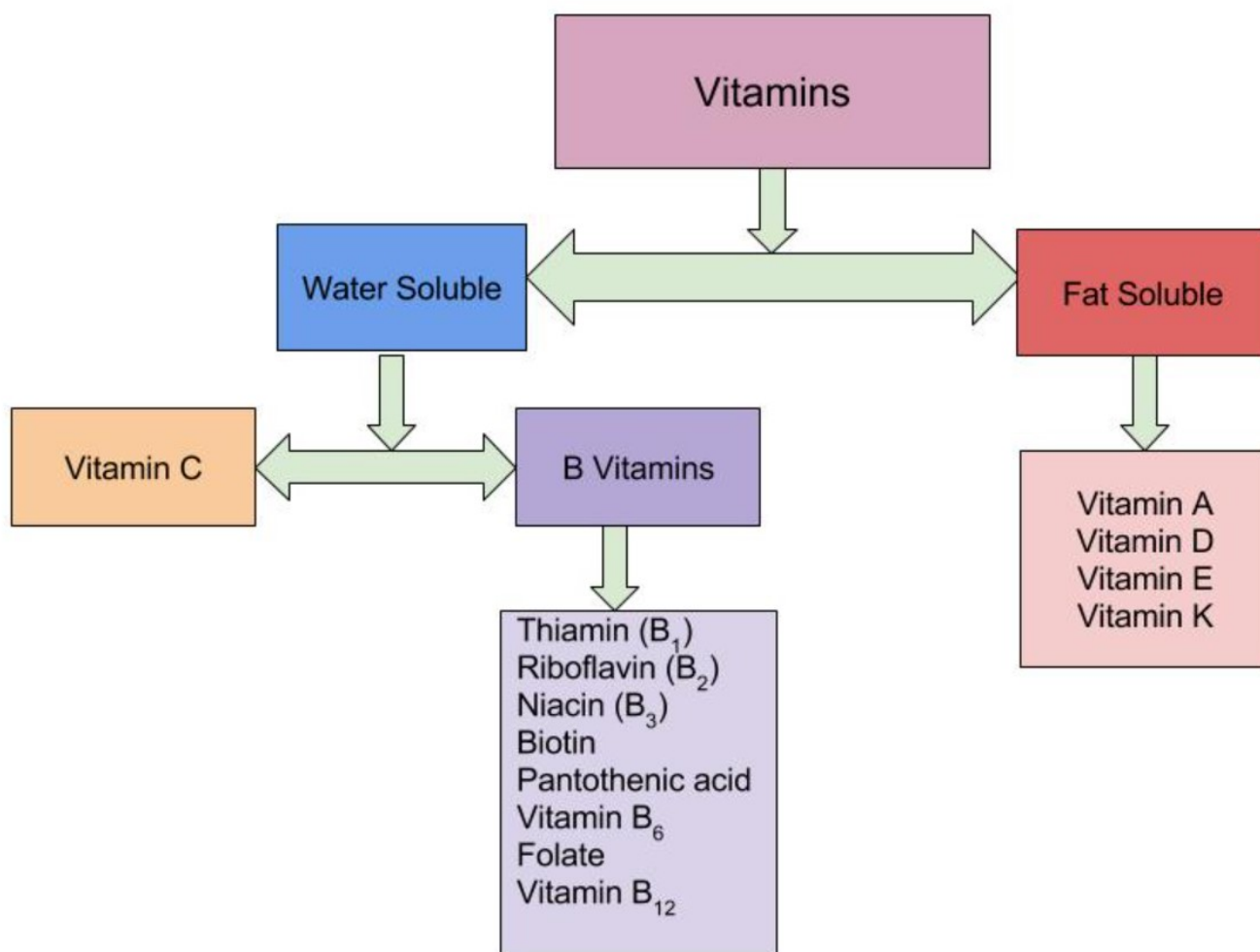


Figure 1.4.4.3: The Vitamins. Image by Allison Calabrese / CC BY 4.0.

Fat Soluble Vitamins

From the structures shown below, it should be clear that these compounds have more than a solubility connection with lipids. Vitamin A is a terpene, and vitamins E and K have long terpene chains attached to an aromatic moiety. The structure of vitamin D can be described as a steroid in which ring B is cut open and the remaining three rings remain unchanged. The precursors of vitamins A and D have been identified as the tetraterpene beta-carotene and the steroid ergosterol, respectively.

Lipid Soluble Vitamins

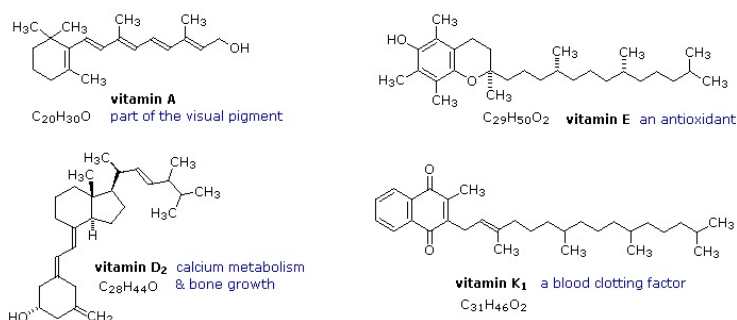


Table 1.4.4.3 lists the different fat soluble vitamins and its function.

Table 1.4.4.3 Fat Soluble Vitamins and Their Function.

Vitamin and alternative name	Sources	Recommended daily allowance	Function	Problems associated with deficiency
A retinal or β -carotene	Yellow and orange fruits and vegetables, dark green leafy vegetables, eggs, milk, liver	700–900 μg	Eye and bone development, immune function	Night blindness, epithelial changes, immune system deficiency
D cholecalciferol	Dairy products, egg yolks; also synthesized in the skin from exposure to sunlight	5–15 μg	Aids in calcium absorption, promoting bone growth	Rickets, bone pain, muscle weakness, increased risk of death from cardiovascular disease, cognitive impairment, asthma in children, cancer
E tocopherols	Seeds, nuts, vegetable oils, avocados, wheat germ	15 mg	Antioxidant	Anemia
K phylloquinone	Dark green leafy vegetables, broccoli, Brussels sprouts, cabbage	90–120 μg	Blood clotting, bone health	Hemorrhagic disease of newborn in infants; uncommon in adults

Web link

More detailed information on the different fat soluble vitamins can be found on the link below.

[https://med.libretexts.org/Bookshelves/Nutrition/Book%3A_Human_Nutrition_\(University_of_Hawaii\)/9%3A_Vitamins/9.2%3A_Fat-Soluble_Vitamins](https://med.libretexts.org/Bookshelves/Nutrition/Book%3A_Human_Nutrition_(University_of_Hawaii)/9%3A_Vitamins/9.2%3A_Fat-Soluble_Vitamins)

Water Soluble Vitamins

All water-soluble vitamins (Table 1.4.4.4) play a different kind of role in energy metabolism; they are required as functional parts of enzymes involved in energy release and storage. Vitamins and minerals that make up part of enzymes are referred to as coenzymes and cofactors, respectively. Coenzymes and cofactors are required by enzymes to catalyze a specific reaction. They assist in converting a substrate to an end-product. Coenzymes and cofactors are essential in catabolic pathways and play a role in many anabolic pathways too. In addition to being essential for metabolism, many vitamins and minerals are required for blood renewal and function. At insufficient levels in the diet these vitamins and minerals impair the health of blood and consequently the delivery of nutrients in and wastes out, amongst its many other functions.

Table 1.4.4.4 *Water Soluble Vitamins and Their Function.*

Vitamin and alternative name	Sources	Recommended daily allowance	Function	Problems associated with deficiency
B ₁ thiamine	Whole grains, enriched bread and cereals, milk, meat	1.1–1.2 mg	Carbohydrate metabolism	Beriberi, Wernicke-Korsikoff syndrome
B ₂ riboflavin	Brewer's yeast, almonds, milk, organ meats, legumes, enriched breads and cereals, broccoli, asparagus	1.1–1.3 mg	Synthesis of FAD for metabolism, production of red blood cells	Fatigue, slowed growth, digestive problems, light sensitivity, epithelial problems like cracks in the corners of the mouth
B ₃ niacin	Meat, fish, poultry, enriched breads and cereals, peanuts	14–16 mg	Synthesis of NAD, nerve function, cholesterol production	Cracked, scaly skin; dementia; diarrhea; also known as pellagra
B ₅ pantothenic acid	Meat, poultry, potatoes, oats, enriched breads and cereals, tomatoes	5 mg	Synthesis of coenzyme A in fatty acid metabolism	Rare: symptoms may include fatigue, insomnia, depression, irritability
B ₆ pyridoxine	Potatoes, bananas, beans, seeds, nuts, meat, poultry, fish, eggs, dark green leafy vegetables, soy, organ meats	1.3–1.5 mg	Sodium and potassium balance, red blood cell synthesis, protein metabolism	Confusion, irritability, depression, mouth and tongue sores
B ₇ biotin	Liver, fruits, meats	30 µg	Cell growth, metabolism of fatty acids, production of blood cells	Rare in developed countries; symptoms include dermatitis, hair loss, loss of muscular coordination
B ₉ folic acid	Liver, legumes, dark green leafy vegetables, enriched breads and cereals, citrus fruits	400 µg	DNA/protein synthesis	Poor growth, gingivitis, appetite loss, shortness of breath, gastrointestinal problems, mental deficits
B ₁₂ cyanocobalamin	Fish, meat, poultry, dairy products, eggs	2.4 µg	Fatty acid oxidation, nerve cell function, red blood cell production	Pernicious anemia, leading to nerve cell damage
C ascorbic acid	Citrus fruits, red berries, peppers, tomatoes, broccoli, dark green leafy vegetables	75–90 mg	Necessary to produce collagen for formation of connective tissue and teeth, and for wound healing	Dry hair, gingivitis, bleeding gums, dry and scaly skin, slow wound healing, easy bruising, compromised immunity; can lead to scurvy

Web link

More detailed information on the different water soluble vitamins can be found on the link below.

Vitamins as Antioxidants

The “big three” vitamin antioxidants are vitamins E, A, and C, although it may be that they are called the “big three” only because they are the most studied. Other antioxidants obtained from the diet are given in Table 1.4.4.5 A simplified diagram on the role of antioxidants is shown in Figure 1.4.4.4

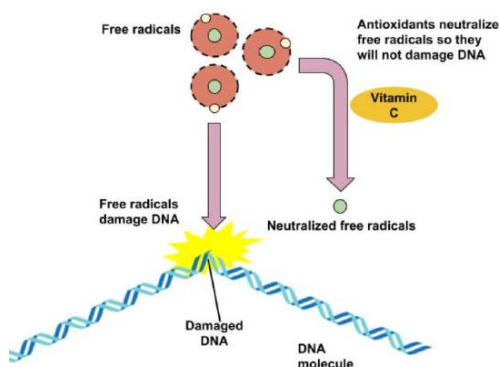


Figure 1.4.4.4 Antioxidants Role. Image: Allison Calabrese / CC BY 4.0

Table 1.4.4.5 *Some Antioxidants Obtained from Diet and Their Related Functions.*

Antioxidant	Functions Attributed to Antioxidant Capacity
Vitamin A	Protects cellular membranes, prevents glutathione depletion, maintains free radical detoxifying enzyme systems, reduces inflammation
Vitamin E	Protects cellular membranes, prevents glutathione depletion
Vitamin C	Protects DNA, RNA, proteins, and lipids, aids in regenerating vitamin E
Carotenoids	Free radical scavengers
Lipoic acid	Free radical scavenger, aids in regeneration of vitamins C and E
Phenolic acids	Free radical scavengers, protect cellular membranes

Effects of Cooking

The USDA has conducted extensive studies on the percentage losses of various nutrients from different food types and cooking methods. Some vitamins may become more “bio-available” – that is, usable by the body – when foods are cooked. Table 1.4.4.6 below shows whether various vitamins are susceptible to loss from heat—such as heat from boiling, steaming, frying, etc. The effect of cutting vegetables can be seen from exposure to air and light. Water-soluble vitamins such as B and C dissolve into the water when a vegetable is boiled, and are then lost when the water is discarded.

Table 1.4.4.6 *Vitamin Stability Upon Air, Light and Heat Exposure. Source: Wikipedia.*

Vitamin	Soluble in Water	Stable to Air Exposure	Stable to Light Exposure	Stable to Heat Exposure
Vitamin A	no	partially	partially	relatively stable
Vitamin C	very unstable	yes	no	no
Vitamin D	no	no	no	no
Vitamin E	no	yes	yes	no
Vitamin K	no	no	yes	no

Vitamin	Soluble in Water	Stable to Air Exposure	Stable to Light Exposure	Stable to Heat Exposure
Thiamine (B ₁)	highly	no	?	> 100 °C
Riboflavin (B ₂)	slightly	no	in solution	no
Niacin (B ₃)	yes	no	no	no
Pantothenic Acid (B ₅)	quite stable	no	no	yes
Vitamin B ₆	yes	?	yes	?
Biotin (B ₇)	somewhat	?	?	no
Folic Acid (B ₉)	yes	?	when dry	at high temp
Cobalamin (B ₁₂)	yes	?	yes	no

Dietary Fiber and Water

Dietary fiber consists of non-starch polysaccharides and other plant components such as cellulose, resistant starch, resistant dextrins, inulin, lignins, chitins, pectins, beta-glucans, and oligosaccharides already mentioned in Section 17.1.

Dietary fibers can act by changing the nature of the contents of the gastrointestinal tract and by changing how other nutrients and chemicals are absorbed. Some types of soluble fiber absorb water to become a gelatinous, viscous substance which may or may not be fermented by bacteria in the digestive tract. Some types of insoluble fiber have bulking action and are not fermented. Lignin, a major dietary insoluble fiber source, may alter the rate and metabolism of soluble fibers. Other types of insoluble fiber, notably resistant starch, are fermented to produce short-chain fatty acids, which are physiologically active and confer health benefits. Health benefit from dietary fiber and whole grains may include a decreased risk of death and lower rates of coronary heart disease, colon cancer, and type 2 diabetes.

Food sources of dietary fiber (Table 1.4.4.7) have traditionally been divided according to whether they provide soluble or insoluble fiber. Plant foods contain both types of fiber in varying amounts, according to the plant's characteristics of viscosity and fermentability. Advantages of consuming fiber depend upon which type of fiber is consumed and which benefits may result in the gastrointestinal system. Bulking fibers – such as cellulose, hemicellulose and psyllium – absorb and hold water, promoting regularity. Viscous fibers – such as beta-glucan and psyllium – thicken the fecal mass. Fermentable fibers – such as resistant starch and inulin – feed the bacteria and microbiota of the large intestine, and are metabolized to yield short-chain fatty acids, which have diverse roles in gastrointestinal health.

Table 1.4.4.7 *Types and Sources of Dietary Fiber.*

Nutrient	Food additive	Source/Comments
Water-insoluble dietary fibers		
β-glucans (a few of which are water-soluble)		
Cellulose	E 460	cereals, fruit, vegetables (in all plants in general)
Chitin	—	in fungi, exoskeleton of insects and crustaceans
Hemicellulose		cereals, bran, timber, legumes
Hexoses	—	wheat, barley
Pentose	—	rye, oat
Lignin	—	stones of fruits, vegetables (filaments of the garden bean), cereals
Xanthan gum	E 415	production with <i>Xanthomonas</i> -bacteria from sugar substrates

Resistant starch		Can be starch protected by seed or shell (type RS1), granular starch (type RS2) or retrograded starch (type RS3)
Resistant starch	—	high amylose corn, barley, high amylose wheat, legumes, raw bananas, cooked and cooled pasta and potatoes
Water-soluble dietary fibers		
Arabinoxylan (a hemicellulose)	—	psyllium
Fructans		replace or complement in some plant taxa the starch as storage carbohydrate
Inulin	—	in diverse plants, e.g. topinambour, chicory, etc.
Polyuronide		
Pectin	E 440	in the fruit skin (mainly apples, quinces), vegetables
Alginic acids(Alginates)	E 400–E 407	in Algae
Sodium alginate	E 401	
Potassium alginate	E 402	
Ammonium alginate	E 403	
Calcium alginate	E 404	
Propylene glycol alginate (PGA)	E 405	
agar	E 406	
carrageen	E 407	red algae
Raffinose	—	legumes
Xylose	—	monosaccharide, pentose
Polydextrose	E 1200	synthetic polymer, ca. 1kcal/g
Lactulose	—	synthetic disaccharide

Fiber Contents in Food

Dietary fibers are found in fruits, vegetables and whole grains. The amount of fiber contained in common foods are in Table 1.4.4.8

Table 1.4.4.8 Amount of Fiber in Common Foods. Source Wikipedia

Food group	Serving mean	Fibermass per serving
Fruit	120 mL (0.5 cup)	1.1 g
Dark green vegetables	120 mL (0.5 cup)	6.4 g
Orange vegetables	120 mL (0.5 cup)	2.1 g
Cooked dry beans (legumes)	120 mL (0.5 cup)	8.0 g
Starchy vegetables	120 mL (0.5 cup)	1.7 g
Other vegetables	120 mL (0.5 cup)	1.1 g

Food group	Serving mean	Fibermass per serving
Whole grains	28 g (1 oz)	2.4 g
Meat	28 g (1 oz)	0.1 g

The breakdown of total dietary fiber in terms of the amounts of soluble and insoluble fiber found in five different foods are listed in Table 1.4.4.9

Table 1.4.4.9 Total Dietary Fiber , Total Nonfermentable Fiber, and Total Fermentable Fiber (as percent of sample weight) in Five Different Foods.

T o t a l D i e t a r y F i b e r	Total Insoluble (Nonfermentable)		Total Soluble (Fermentable)	
C e r e a l , a l l b r a n	3 0 . 1	28.0	2.1	

B l u e b e r r i e s , f r e s h	2 . 2.4 7	0.3	
B r o c c o l i , f r e s h , c o o k e d	3 . 3.1 5	0.4	

P o r k a n d b e a n s , c a n n e d	4 . 3.0 4	1.4
A l m o n d s , w i t h s k i n	8 . 8.6 8	0.2

tr = trace amounts

Dietary fiber is found in plants, typically eaten whole, raw or cooked, although fiber can be added to make dietary supplements and fiber-rich processed foods. Grain bran products have the highest fiber contents, such as crude corn bran (79 g per 100 g) and crude wheat bran (43 g per 100 g), which are ingredients for manufactured foods. Medical authorities, such as the Mayo Clinic, recommend adding fiber-rich products to the Standard American Diet (SAD) which is rich in processed and artificially sweetened foods, with minimal intake of vegetables and legumes.

Plant Sources of Fiber

Some plants contain significant amounts of soluble and insoluble fiber. For example, plums and prunes have a thick skin covering a juicy pulp. The skin is a source of insoluble fiber, whereas soluble fiber is in the pulp. Grapes also contain a fair amount of fiber. A listing of other plant sources of fiber is given in the table below.

Table 1.4.4.10 *Plant Sources of Soluble and Insoluble Fiber.*

Sources of Soluble Fiber	Sources of Insoluble Fiber

- legumes (peas, soybeans, lupins and other beans)
- oats, rye, chia, and barley
- some fruits (including figs, avocados, plums, prunes, berries, ripe bananas, and the skin of apples, quinces and pears)
- certain vegetables such as broccoli, carrots, and Jerusalem artichokes
- root tubers and root vegetables such as sweet potatoes and onions (skins of these are sources of insoluble fiber also)
- psyllium seed husks (a mucilage soluble fiber) and flax seeds
- nuts, with almonds being the highest in dietary fiber
- whole grain foods
- wheat and corn bran
- legumes such as beans and peas
- nuts and seeds
- potato skins
- lignans
- vegetables such as green beans, cauliflower, zucchini (courgette), celery, and nopal
- some fruits including avocado, and unripe bananas
- the skins of some fruits, including kiwifruit, grapes and tomatoes

Fiber Supplements

These are a few example forms of fiber that have been sold as supplements or food additives. These may be marketed to consumers for nutritional purposes, treatment of various gastrointestinal disorders, and for such possible health benefits as lowering cholesterol levels, reducing risk of colon cancer, and losing weight.

Soluble fiber supplements may be beneficial for alleviating symptoms of irritable bowel syndrome, such as diarrhea or constipation and abdominal discomfort. Prebiotic soluble fiber products, like those containing inulin or oligosaccharides, may contribute to relief from inflammatory bowel disease, as in Crohn's disease, ulcerative colitis, and *Clostridium difficile*, due in part to the short-chain fatty acids produced with subsequent anti-inflammatory actions upon the bowel. Fiber supplements may be effective in an overall dietary plan for managing irritable bowel syndrome by modification of food choices.

One insoluble fiber, resistant starch from high-amylose corn, has been used as a supplement and may contribute to improving insulin sensitivity and glycemic management as well as promoting regularity and possibly relief of diarrhea. One preliminary finding indicates that resistant corn starch may reduce symptoms of ulcerative colitis.

Inulin

Chemically defined as oligosaccharides occurring naturally in most plants, inulins have nutritional value as carbohydrates, or more specifically as fructans, a polymer of the natural plant sugar, fructose. Inulin is typically extracted by manufacturers from enriched plant sources such as chicory roots or Jerusalem artichokes for use in prepared foods. Subtly sweet, it can be used to replace sugar, fat, and flour, is often used to improve the flow and mixing qualities of powdered nutritional supplements, and has significant potential health value as a prebiotic fermentable fiber.

Inulin is advantageous because it contains 25–30% the food energy of sugar or other carbohydrates and 10–15% the food energy of fat. As a prebiotic fermentable fiber, its metabolism by gut flora yields short-chain fatty acids (see below) which increase absorption of calcium, magnesium, and iron, resulting from upregulation of mineral-transporting genes and their membrane transport proteins within the colon wall. Among other potential beneficial effects noted above, inulin promotes an increase in the mass and health of intestinal *Lactobacillus* and *Bifidobacterium* populations.

Inulin's primary disadvantage is its tolerance. As a soluble fermentable fiber, it is quickly and easily fermented within the intestinal tract, which may cause gas and digestive distress at doses higher than 15 grams/day in most people. Individuals with digestive diseases have benefited from removing fructose and inulin from their diet. While clinical studies have shown changes in the microbiota at lower levels of inulin intake, some of the health effects require higher than 15 grams per day to achieve the benefits.

Vegetable Gums

Vegetable gum fiber supplements are relatively new to the market. Often sold as a powder, vegetable gum fibers dissolve easily with no aftertaste. In preliminary clinical trials, they have proven effective for the treatment of irritable bowel syndrome. Examples of vegetable gum fibers are guar gum and gum arabic.

Water

Add all the ways you use water every day and you still will not come close to the countless uses water has in the human body. Of all the nutrients, water is the most critical as its absence proves lethal within a few days. Organisms have adapted numerous mechanisms for water conservation. Water uses in the human body can be loosely categorized into four basic functions: transportation vehicle, medium for chemical reactions, lubricant/shock absorber, and temperature regulator.

On a typical day, the average adult will take in about 2500 mL (almost 3 quarts) of aqueous fluids. Although most of the intake comes through the digestive tract, about 230 mL (8 ounces) per day is generated metabolically, in the last steps of aerobic respiration. Additionally, each day about the same volume (2500 mL) of water leaves the body by different routes; most of this lost water is removed as urine. The kidneys also can adjust blood volume through mechanisms that draw water out of the filtrate and urine. The kidneys can regulate water levels in the body; they conserve water if you are dehydrated, and they can make urine more dilute to expel excess water if necessary. Water is lost through the skin through evaporation from the skin surface without overt sweating and from air expelled from the lungs. This type of water loss is called insensible water loss because a person is usually unaware of it.

Summary

- Vitamins and minerals are essential parts of the diet. They are needed for the proper function of metabolic pathways in the body.
- Vitamins are not stored in the body, so they must be obtained from the diet or synthesized from precursors available in the diet.
- Minerals are also obtained from the diet, but they are also stored, primarily in skeletal tissues.
- Dietary fibers can act by changing the nature of the contents of the gastrointestinal tract and by changing how other nutrients and chemicals are absorbed.
- Whole grain, legumes, vegetables, and fruits are excellent sources of dietary fiber.
- Health benefit from dietary fiber and whole grains may include a decreased risk of death and lower rates of coronary heart disease, colon cancer, and type 2 diabetes.

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CHAPTER OVERVIEW

2: Chemicals in Water

2.1: Types of Bonds

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2.1.2: Forces in Solutions

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2.1: Types of Bonds

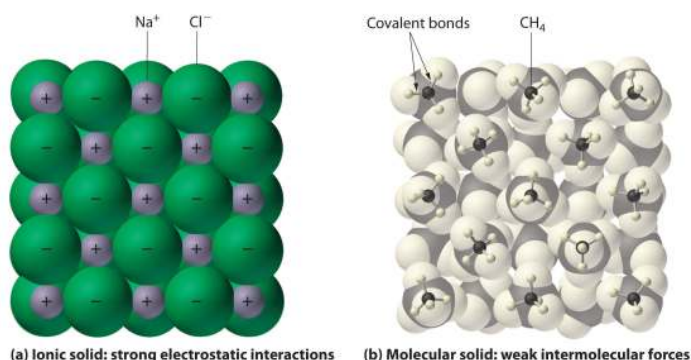
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2.1.1: Comparing Ionic and Molecular Substances

Learning Objectives

- Know the physical properties of ionic and molecular substances.

The physical state and properties of a particular compound depend in large part on the type of chemical bonding it displays. **Molecular compounds**, sometimes called



(a) The positively and negatively charged ions in an ionic solid such as sodium chloride (NaCl) are held together by strong electrostatic interactions. (b) In this representation of the packing of methane (CH_4) molecules in solid methane, a prototypical molecular solid, the methane molecules are held together in the solid only by relatively weak intermolecular forces, even though the atoms within each methane molecule are held together by strong covalent bonds.

covalent compounds, display a wide range of physical properties due to the different types of intermolecular attractions such as different kinds of polar interactions. The melting and boiling points of molecular compounds are generally quite low compared to those of **ionic compounds**. This is because the energy required to disrupt the **intermolecular forces** between molecules is far less than the energy required to break the ionic bonds in a crystalline ionic compound (Figure 2.1.1.1). Ionic solids typically melt at high temperatures and boil at even higher temperatures. For example, sodium chloride melts at 801°C and boils at 1413°C . (As a comparison, the molecular compound water melts at 0°C and boils at 100°C .) The water solubility of molecular compounds is variable and depends primarily on the type of intermolecular forces involved.

Figure 2.1.1.1 Interactions in Ionic and Covalent Solids.

Since molecular compounds are composed of neutral molecules, their electrical conductivity is generally quite poor, whether in the solid or liquid state. In solid form, an ionic compound is not electrically conductive because its ions are unable to flow ("electricity" is the flow of charged particles). When molten, however, it can conduct electricity because its ions are able to move freely through the liquid (Figure 2.1.1.2 Video 2.1.1.1).

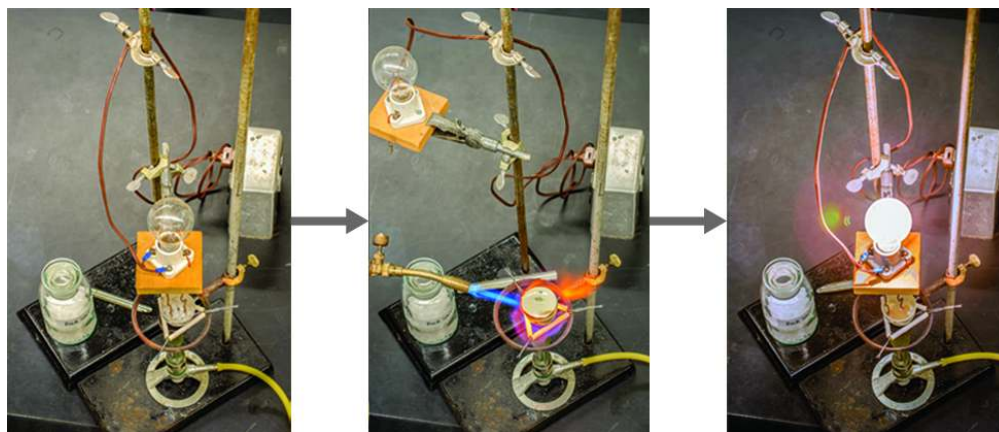


Figure 2.1.1.2 Sodium chloride melts at 801 °C and conducts electricity when molten. (credit: modification of work by Mark Blaser and Matt Evans)

This figure shows three photos connected by right-facing arrows. The first shows a light bulb as part of a complex lab equipment setup. The light bulb is not lit. The second photo shows a substance being heated or set on fire. The third shows the light bulb again which is lit.

Conductivity of Molten Salt



Video 2.1.1.1 Watch this video to see a mixture of salts melt and conduct electricity.

The table below summarizes some of the differences between ionic and molecular compounds.

Table 2.1.1.1 Comparison of Ionic and Molecular Compounds

Property	Ionic Compounds	Molecular Compounds
Type of elements	Metal and nonmetal	Nonmetals only
Bonding	Ionic - transfer of electron(s) between atoms	Covalent - sharing of pair(s) of electrons between atoms
Representative unit	Formula unit	Molecule
Physical state at room temperature	Solid	Gas, liquid, or solid
Water solubility	Usually high	Variable
Melting and boiling temperatures	Generally high	Generally low
Electrical conductivity	Good when molten or in solution	Poor

One type of molecular compound behaves quite differently than that described so far. A covalent network solid is a compound in which all of the atoms are connected to one another by covalent bonds. Diamond is composed entirely of carbon atoms, each

bonded to four other carbon atoms in a tetrahedral geometry. Melting a covalent network solid is not accomplished by overcoming the relatively weak intermolecular forces. Rather, all of the covalent bonds must be broken, a process that requires extremely high temperatures. Diamond, in fact, does not melt at all. Instead, it vaporizes to a gas at temperatures above 3500°C.

Summary

- The physical properties of a material are affected by the intermolecular forces holding the molecules together.
- Ionic compounds usually form hard crystalline solids with high melting points. Covalent molecular compounds, in contrast, consist of discrete molecules held together by weak intermolecular forces and can be gases, liquids, or solids at room temperature and pressure.
- Ionic compounds in molten form or in solution can conduct electricity while molecular compounds do not..

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2.1.2: Forces in Solutions

Learning Objectives

- Learn some terminology involving solutions.
- Explain the significance of the statement "like dissolves like".
- Explain why certain substances dissolve in other substances.

A **solution** is another name for a homogeneous mixture. A **mixture** is a material composed of two or more substances. In a solution, the combination is so intimate that the



Figure 2.1.2.1 Making a saline water solution by dissolving table salt (NaCl) in water. The salt is the solute and the water the solvent. (CC-BY-SA 3.0; Chris 73).

different substances cannot be differentiated by sight, even with a microscope. Compare, for example, a mixture of salt and pepper and another mixture consisting of salt and water. In the first mixture, we can readily see individual grains of salt and the flecks of pepper. A mixture of salt and pepper is not a solution. However, in the second mixture, no matter how carefully we look, we cannot see two different substances. Salt dissolved in water is a solution.

The major component of a solution, called the **solvent**, is typically the same phase as the solution itself. Each minor component of a solution (and there may be more than one) is called the **solute**. In most of the solutions we will describe in this textbook, there will be no ambiguity about whether a component is the solvent or the solute.) For example, in a solution of salt in water, the solute is salt, and solvent is water Figure 2.1.2.1.

Solutions come in all phases, and the solvent and the solute do not have to be in the same phase to form a solution (such as salt and water). For example, air is a gaseous solution of about 80% nitrogen and about 20% oxygen, with some other gases present in much smaller amounts. An alloy is a solid solution consisting of a metal (like iron) with some other metals or nonmetals dissolved in it. Steel, an alloy of iron and carbon and small amounts of other metals, is an example of a solid solution. Table 2.1.2.1 lists some common types of solutions, with examples of each.

Table 2.1.2.1 Types of Solutions

Solvent Phase	Solute Phase	Example
gas	gas	air
liquid	gas	carbonated beverages
liquid	liquid	ethanol (C ₂ H ₅ OH) in H ₂ O (alcoholic beverages)
liquid	solid	salt water
solid	gas	H ₂ gas absorbed by Pd metal
solid	liquid	Hg(l) in dental fillings
solid	solid	steel alloys

✓ Example 2.1.2.1: Sugar and Water

A solution is made by dissolving 1.00 g of sucrose ($C_{12}H_{22}O_{11}$) in 100.0 g of liquid water. Identify the solvent and solute in the resulting solution.

Solution

Either by mass or by moles, the obvious minor component is **sucrose**, so it is **the solute**. **Water**—the majority component—is **the solvent**. The fact that the resulting solution is the same phase as water also suggests that water is the solvent.

? Exercise 2.1.2.1

A solution is made by dissolving 3.33 g of $HCl(g)$ in 40.0 g of liquid methyl alcohol (CH_3OH). Identify the solvent and solute in the resulting solution.

Answer

solute: $HCl(g)$; solvent: CH_3OH

Like Dissolves Like

A simple way to predict which compounds will dissolve in other compounds is the phrase "like dissolves like". What this means is that polar compounds dissolve polar compounds, nonpolar compounds dissolve nonpolar compounds, but polar and nonpolar do not dissolve in each other.

Even some nonpolar substances dissolve in water but only to a limited degree. Have you ever wondered why fish are able to breathe? Oxygen gas, an nonpolar molecules, does dissolve in water and it is this oxygen that the fish take in through their gills. Or, one more example of a nonpolar compound that dissolves in water is the reason we can enjoy carbonated sodas. Pepsi-cola and all the other sodas have carbon dioxide gas, CO_2 , a nonpolar compound, dissolved in a sugar-water solution. In this case, to keep as much gas in solution as possible, the sodas are kept under pressure.

This general trend of "like dissolves like" is summarized in the following table:

Table 2.1.2.2 Summary of Solubilities

Solute	Solvent	Is Solution Formed?
Polar Covalent	Polar	yes
Non-polar Covalent	Non-polar	yes
Polar Covalent	Non-polar	no
Non-polar Covalent	Polar	no
Ionic	Polar	yes
Ionic	Non-polar	no

Note that every time charged particles (ionic compounds or polar substances) are mixed, a solution is formed. When particles with no charges (nonpolar compounds) are mixed, they will form a solution. However, if substances with charges are mixed with other substances without charges a solution does not form.

When an ionic compound is considered "insoluble", it doesn't necessarily mean the compound is completely untouched by water. All ionic compounds dissolve to some extent. An insoluble compound just doesn't dissolve in any noticeable or appreciable amount.

What is it that makes a solute soluble in some solvents but not others?

The answer is intermolecular interactions. The intermolecular interactions include London dispersion forces, dipole-dipole interactions, and hydrogen bonding (as described in



Figure 2.1.2.1 Making a saline water solution by dissolving table salt (NaCl) in water. The salt is the solute and the water the solvent. (CC-BY-SA 3.0; Chris 73).

the previous section). From experimental studies, it has been determined that if molecules of a solute experience the same intermolecular forces that the solvent does, the solute will likely dissolve in that solvent. So, NaCl—a very polar substance because it is composed of ions—dissolves in water, which is very polar, but not in oil, which is generally nonpolar. Nonpolar wax dissolves in nonpolar hexane, but not in polar water. *Liquids that dissolve in one another in all proportions are said to be **miscible**. Liquids that do not dissolve in one another are called **immiscible**.*

Figure 2.1.2.2 Water (clear liquid) and oil (yellow) do not form liquid solutions. (CC BY-SA 1.0 Generic; Victor Blacus)

✓ Example 2.1.2.2: Polar and Nonpolar Solvents

Would I₂ be more soluble in CCl₄ or H₂O? Explain your answer.

Solution

I₂ is nonpolar. Of the two solvents, CCl₄ is nonpolar and H₂O is polar, so I₂ would be expected to be more soluble in CCl₄.

? Exercise 2.1.2.2

Would C₃H₇OH be more soluble in CCl₄ or H₂O? Explain your answer.

Answer

H₂O because both experience hydrogen bonding

✓ Example 2.1.2.3

Water is considered a polar solvent. Which substances should dissolve in water?

- methanol (CH₃OH)
- sodium sulfate (Na₂SO₄)
- octane (C₈H₁₈)

Solution

Because water is polar, substances that are polar or ionic will dissolve in it.

- Because of the OH group in methanol, we expect its molecules to be polar. Thus, we expect it to be soluble in water. As both water and methanol are liquids, the word *miscible* can be used in place of *soluble*.
- Sodium sulfate is an ionic compound, so we expect it to be soluble in water.
- Like other hydrocarbons, octane is nonpolar, so we expect that it would not be soluble in water.

? Exercise 2.1.2.3

Toluene ($\text{C}_6\text{H}_5\text{CH}_3$) is widely used in industry as a nonpolar solvent. Which substances should dissolve in toluene?

- water (H_2O)
- sodium sulfate (Na_2SO_4)
- octane (C_8H_{18})

Answer

octane (C_8H_{18}) will dissolve. It is also non-polar.

The Dissolving Process

Water typically dissolves most ionic compounds and polar molecules. Nonpolar molecules, such as those found in grease or oil, do not dissolve in water. We will first examine the process that occurs when an ionic compound, such as table salt (sodium chloride), dissolves in water.

Water molecules move about continuously due to their kinetic energy. When a crystal of sodium chloride is placed into water, the water's molecules collide with the crystal lattice. Recall that the crystal lattice is composed of alternating positive and negative ions. Water is attracted to the sodium chloride crystal because water is polar; it has both a positive and a negative end. The positively charged sodium ions in the crystal attract the oxygen end of the water molecules because they are partially negative. The negatively charged chloride ions in the crystal attract the hydrogen end of the water molecules because they are partially positive. The action of the polar water molecules takes the crystal lattice apart (see figure below).

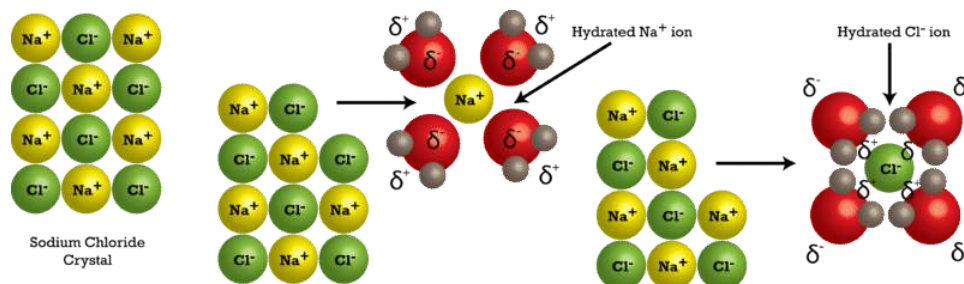


Figure 2.1.2.3: The process of an ionic sodium chloride crystal being dissolved and hydrated by water.

After coming apart from the crystal, the individual ions are then surrounded by solvent particles in a process called **solvation**. Note in the figure above that the individual Na^+ ions are surrounded by water molecules with the oxygen atom oriented near the positive ion. Likewise, the chloride ions are surrounded by water molecules with the opposite orientation. Thus, numerous **ion-dipole** interactions are formed. **Hydration** is the process of solute particles being surrounded by water molecules arranged in a specific manner. Hydration helps to stabilize aqueous solutions by preventing the positive and negative ions from coming back together and forming a precipitate.

Table sugar is made of the molecular compound sucrose ($\text{C}_{12}\text{H}_{22}\text{O}_{11}$). Solid sugar consists of individual sugar molecules held together by intermolecular attractive forces. When water dissolves sugar, it separates the individual sugar molecules by disrupting the attractive forces, but it *does not break the covalent bonds* between the carbon, hydrogen, and oxygen atoms. Dissolved sugar molecules are also hydrated. The hydration shell around a molecule of sucrose is arranged so that its partially negative oxygen atoms are near the partially positive hydrogen atoms in the solvent, and vice versa.

Summary

- Solutions are composed of a solvent (major component) and a solute (minor component).
- “Like dissolves like” is a useful rule for deciding if a solute will be soluble in a solvent.
- Liquids that dissolve in one another in all proportions are said to be **miscible**.
- Liquids that do not dissolve in one another are called **immiscible**.
- Ion-dipole** interactions are formed when ionic compounds dissolve in water.

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2.2: How Molecules Dissolve

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2.2.1: The Dissolution Process

Learning Objectives

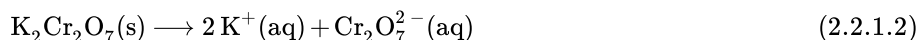
- Describe the basic properties of solutions and how they form.
- Predict whether a given mixture will yield a solution based on molecular properties of its components.
- Explain why some solutions either produce or absorb heat when they form.

An earlier chapter of this text introduced *solutions*, defined as homogeneous mixtures of two or more substances. Often, one component of a solution is present at a significantly greater concentration, in which case it is called the solvent. The other components of the solution present in relatively lesser concentrations are called solutes. Sugar is a covalent solid composed of sucrose molecules, $C_{12}H_{22}O_{11}$. When this compound dissolves in water, its molecules become uniformly distributed among the molecules of water:



The subscript “aq” in the equation signifies that the sucrose molecules are solutes and are therefore *individually dispersed* throughout the *aqueous solution* (water is the solvent). Although sucrose molecules are heavier than water molecules, they remain dispersed throughout the solution; gravity does not cause them to “settle out” over time.

Potassium dichromate, $K_2Cr_2O_7$, is an ionic compound composed of colorless potassium ions, K^+ , and orange dichromate ions, $Cr_2O_7^{2-}$. When a small amount of solid potassium dichromate is added to water, the compound dissolves and dissociates to yield potassium ions and dichromate ions uniformly distributed throughout the mixture (Figure 2.2.1.1), as indicated in this equation:



As with the mixture of sugar and water, this mixture is also an aqueous solution. Its solutes, potassium and dichromate ions, remain individually dispersed among the solvent (water) molecules.



Figure 2.2.1.1: When potassium dichromate ($K_2Cr_2O_7$) is mixed with water, it forms a homogeneous orange solution. (credit: modification of work by Mark Ott)

The first photo shows a small mound of an orange crystalline solid. There is a right-facing arrow. The second photo shows a translucent, colorless liquid in a clear container. There is a right-facing arrow. The third photo shows a translucent orange liquid in a clear, covered container.

Water is used so often as a solvent that the word solution has come to imply an aqueous solution to many people. However, almost any gas, liquid, or solid can act as a solvent. Many alloys are solid solutions of one metal dissolved in another; for example, US five-cent coins contain nickel dissolved in copper. Air is a gaseous solution, a homogeneous mixture of nitrogen, oxygen, and several other gases. Oxygen (a gas), alcohol (a liquid), and sugar (a solid) all dissolve in water (a liquid) to form liquid solutions. Table 2.2.1.1 gives examples of several different solutions and the phases of the solutes and solvents.

Table 2.2.1.1: Different Types of Solutions

Solution	Solute	Solvent
air	$O_2(g)$	$N_2(g)$
soft drinks	$CO_2(g)$	$H_2O(l)$
hydrogen in palladium	$H_2(g)$	$Pd(s)$
rubbing alcohol	$H_2O(l)$	$C_3H_8O(l)$ (2-propanol)
saltwater	$NaCl(s)$	$H_2O(l)$

Solution	Solute	Solvent
brass	Zn(s)	Cu(s)

Solutions exhibit these defining traits:

- They are homogeneous; that is, after a solution is mixed, it has the same composition at all points throughout (its composition is uniform).
- The physical state of a solution—solid, liquid, or gas—is typically the same as that of the solvent, as demonstrated by the examples in Table 2.2.1.1.
- The components of a solution are dispersed on a molecular scale; that is, they consist of a mixture of separated molecules, atoms, and/or ions.
- The dissolved solute in a solution will not settle out or separate from the solvent.
- The composition of a solution, or the concentrations of its components, can be varied continuously, within limits.

The Formation of Solutions

The formation of a solution is an example of a spontaneous process, a process that occurs under specified conditions without the requirement of energy from some external source. Sometimes we stir a mixture to speed up the dissolution process, but this is not necessary; a homogeneous solution would form if we waited long enough. The topic of spontaneity is critically important to the study of chemical thermodynamics and is treated more thoroughly in a later chapter of this text. For purposes of this chapter's discussion, it will suffice to consider two criteria that *favor*, but do not guarantee, the spontaneous formation of a solution:

1. a decrease in the internal energy of the system (an exothermic change, as discussed in the previous chapter on thermochemistry)
2. an increase in the disorder in the system (which indicates an increase in the *entropy* of the system, as you will learn about in the later chapter on thermodynamics)

In the process of dissolution, an internal energy change often, but not always, occurs as heat is absorbed or evolved. An increase in disorder always results when a solution forms.

When the strengths of the intermolecular forces of attraction between solute and solvent species in a solution are no different than those present in the separated components, the solution is formed with no accompanying energy change. Such a solution is called an ideal solution. A mixture of ideal gases (or gases such as helium and argon, which closely approach ideal behavior) is an example of an ideal solution, since the entities comprising these gases experience no significant intermolecular attractions.

When containers of helium and argon are connected, the gases spontaneously mix due to diffusion and form a solution (Figure 2.2.1.2). The formation of this solution clearly involves an increase in disorder, since the helium and argon atoms occupy a volume twice as large as that which each occupied before mixing.

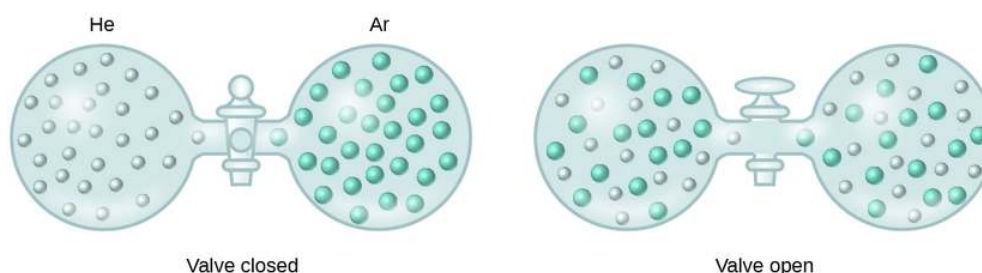


Figure 2.2.1.2: Samples of helium and argon spontaneously mix to give a solution in which the disorder of the atoms of the two gases is increased.

Two figures are shown. The first contains two spherical containers joined by a closed stopcock. The container to the left is labeled H e. It holds about thirty evenly dispersed, small, light blue spheres. The container on the right is labeled A r and contains about thirty slightly larger blue-green spheres. The second, similar figure has an open stopcock between the two spherical containers. The light blue and green spheres are evenly dispersed and present in both containers.

Ideal solutions may also form when structurally similar liquids are mixed. For example, mixtures of the alcohols methanol (CH_3OH) and ethanol ($\text{C}_2\text{H}_5\text{OH}$) form ideal solutions, as do mixtures of the hydrocarbons pentane, C_5H_{12} , and hexane, C_6H_{14} . Placing methanol and ethanol, or pentane and hexane, in the bulbs shown in Figure 2.2.1.2 will result in the same diffusion and subsequent mixing of these liquids as is observed for the He and Ar gases (although at a much slower rate), yielding solutions with no significant change in energy. Unlike a mixture of gases, however, the components of these liquid-liquid solutions do, indeed,

experience intermolecular attractive forces. But since the molecules of the two substances being mixed are structurally very similar, the intermolecular attractive forces between like and unlike molecules are essentially the same, and the dissolution process, therefore, does not entail any appreciable increase or decrease in energy. These examples illustrate how diffusion alone can provide the driving force required to cause the spontaneous formation of a solution. In some cases, however, the relative magnitudes of intermolecular forces of attraction between solute and solvent species may prevent dissolution.

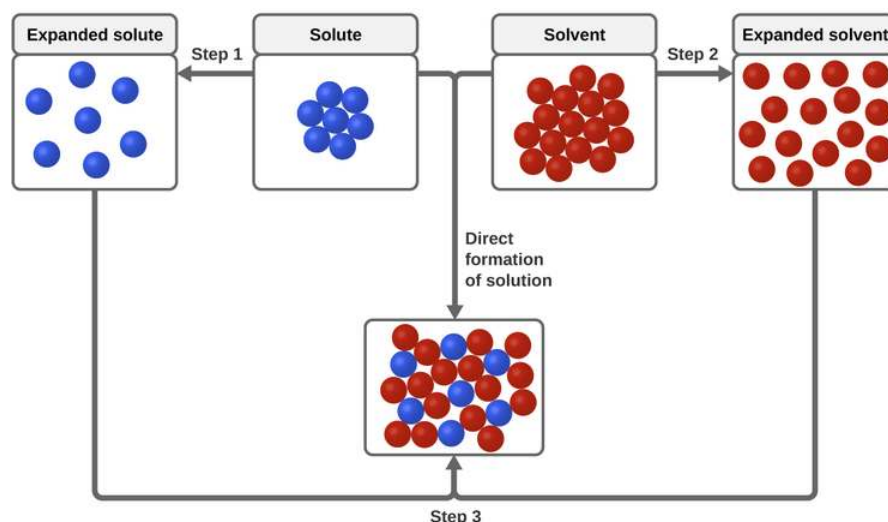


Figure 2.2.1.3: This schematic representation of dissolution shows a stepwise process involving the endothermic separation of solute and solvent species (Steps 1 and 2) and exothermic solvation (Step 3).

The top, central region of the figure shows solute particles as seven blue spheres and solvent particles as 16 red spheres in separate, labeled boxes. The particles in these boxes are touching. An arrow labeled “Step 1” points left of the solute box, and shows the blue spheres no longer touching in another box labeled “expanded solute.” An arrow labeled “Step 2” points right from the solvent box and shows the red spheres no longer touching in another box labeled “expanded solvent.” Arrows proceed from the bottom of the expanded solute and expanded solvent boxes and join at the bottom of the figure where a step 3 label is shown. The joined arrows point to a box just above in which the red and blue spheres are mixed together and touching. The solute and solvent boxes are joined by another arrow labeled “direct formation of solution” which points downward at the center of the figure. This arrow also points to the box containing mixed red and blue spheres near the bottom of the figure.

Three types of intermolecular attractive forces are relevant to the dissolution process: solute-solute, solvent-solvent, and solute-solvent. As illustrated in Figure 2.2.1.3 the formation of a solution may be viewed as a stepwise process in which energy is consumed to overcome solute-solute and solvent-solvent attractions (endothermic processes) and released when solute-solvent attractions are established (an exothermic process referred to as solvation). The relative magnitudes of the energy changes associated with these stepwise processes determine whether the dissolution process overall will release or absorb energy. In some cases, solutions do not form because the energy required to separate solute and solvent species is so much greater than the energy released by solvation.



Figure 2.2.1.4: A mixture of nonpolar cooking oil and polar water does not yield a solution. (credit: Gautam Dogra).

For example, cooking oils and water will not mix to any appreciable extent to yield solutions (Figure 2.2.1.4). Hydrogen bonding is the dominant intermolecular attractive force present in liquid water; the nonpolar hydrocarbon molecules of cooking oils are not

capable of hydrogen bonding, instead being held together by dispersion forces. Forming an oil-water solution would require overcoming the very strong hydrogen bonding in water, as well as the significantly strong dispersion forces between the relatively large oil molecules. And, since the polar water molecules and nonpolar oil molecules would not experience very strong intermolecular attraction, very little energy would be released by solvation.

On the other hand, a mixture of ethanol and water will mix in any proportions to yield a solution. In this case, both substances are capable of hydrogen bonding, and so the solvation process is sufficiently exothermic to compensate for the endothermic separations of solute and solvent molecules.



Figure 2.2.1.5: An instant cold pack gets cold when certain salts, such as ammonium nitrate, dissolve in water—an endothermic process.

This figure shows a single use instant cold pack with labels indicating an inner bag of water surrounded by white particulate ammonium nitrate.

As noted at the beginning of this module, spontaneous solution formation is favored, but not guaranteed, by exothermic dissolution processes. While many soluble compounds do, indeed, dissolve with the release of heat, some dissolve endothermically. Ammonium nitrate (NH_4NO_3) is one such example and is used to make instant cold packs for treating injuries like the one pictured in Figure 2.2.1.5. A thin-walled plastic bag of water is sealed inside a larger bag with solid NH_4NO_3 . When the smaller bag is broken, a solution of NH_4NO_3 forms, absorbing heat from the surroundings (the injured area to which the pack is applied) and providing a cold compress that decreases swelling. Endothermic dissolutions such as this one require a greater energy input to separate the solute species than is recovered when the solutes are solvated, but they are spontaneous nonetheless due to the increase in disorder that accompanies formation of the solution.



Video 2.2.1.1: Watch this brief video illustrating endothermic and exothermic dissolution processes.

Summary

A solution forms when two or more substances combine physically to yield a mixture that is homogeneous at the molecular level. The solvent is the most concentrated component and determines the physical state of the solution. The solutes are the other components typically present at concentrations less than that of the solvent. Solutions may form endothermically or exothermically, depending upon the relative magnitudes of solute and solvent intermolecular attractive forces. Ideal solutions form with no appreciable change in energy.

Footnotes

1. If bubbles of gas are observed within the liquid, the mixture is not homogeneous and, thus, not a solution.

Glossary

alloy

solid mixture of a metallic element and one or more additional elements

ideal solution

solution that forms with no accompanying energy change

solvation

exothermic process in which intermolecular attractive forces between the solute and solvent in a solution are established

spontaneous process

physical or chemical change that occurs without the addition of energy from an external source

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2.2.2: Molarity

Learning Objectives

- Describe the fundamental properties of solutions
- Calculate solution concentrations using molarity
- Perform dilution calculations using the dilution equation

In preceding sections, we focused on the composition of substances: samples of matter that contain only one type of element or compound. However, mixtures—samples of matter containing two or more substances physically combined—are more commonly encountered in nature than are pure substances. Similar to a pure substance, the relative composition of a mixture plays an important role in determining its properties. The relative amount of oxygen in a planet’s atmosphere determines its ability to sustain aerobic life. The relative amounts of iron, carbon, nickel, and other elements in steel (a mixture known as an “alloy”) determine its physical strength and resistance to corrosion. The relative amount of the active ingredient in a medicine determines its effectiveness in achieving the desired pharmacological effect. The relative amount of sugar in a beverage determines its sweetness (Figure 2.2.2.1). In this section, we will describe one of the most common ways in which the relative compositions of mixtures may be quantified.



Figure 2.2.2.1: Sugar is one of many components in the complex mixture known as coffee. The amount of sugar in a given amount of coffee is an important determinant of the beverage’s sweetness. (credit: Jane Whitney)

Solutions

We have previously defined solutions as homogeneous mixtures, meaning that the composition of the mixture (and therefore its properties) is uniform throughout its entire volume. Solutions occur frequently in nature and have also been implemented in many forms of manmade technology. We will explore a more thorough treatment of solution properties in the chapter on solutions and colloids, but here we will introduce some of the basic properties of solutions.

The relative amount of a given solution component is known as its concentration. Often, though not always, a solution contains one component with a concentration that is significantly greater than that of all other components. This component is called the solvent and may be viewed as the medium in which the other components are dispersed, or dissolved. Solutions in which water is the solvent are, of course, very common on our planet. A solution in which water is the solvent is called an aqueous solution.

A solute is a component of a solution that is typically present at a much lower concentration than the solvent. Solute concentrations are often described with qualitative terms such as dilute (of relatively low concentration) and concentrated (of relatively high concentration).

Concentrations may be quantitatively assessed using a wide variety of measurement units, each convenient for particular applications. Molarity (M) is a useful concentration unit for many applications in chemistry. Molarity is defined as the number of moles of solute in exactly 1 liter (1 L) of the solution:

$$M = \frac{\text{mol solute}}{\text{L solution}} \quad (2.2.2.1)$$

✓ Example 2.2.2.1: Calculating Molar Concentrations

A 355-mL soft drink sample contains 0.133 mol of sucrose (table sugar). What is the molar concentration of sucrose in the beverage?

Solution

Since the molar amount of solute and the volume of solution are both given, the molarity can be calculated using the definition of molarity. Per this definition, the solution volume must be converted from mL to L:

$$\begin{aligned} M &= \frac{\text{mol solute}}{\text{L solution}} \\ &= \frac{0.133 \text{ mol}}{355 \text{ mL} \times \frac{1 \text{ L}}{1000 \text{ mL}}} \\ &= 0.375 \text{ M} \end{aligned}$$

? Exercise 2.2.2.1

A teaspoon of table sugar contains about 0.01 mol sucrose. What is the molarity of sucrose if a teaspoon of sugar has been dissolved in a cup of tea with a volume of 200 mL?

Answer

0.05 M

✓ Example 2.2.2.2: Deriving Moles and Volumes from Molar Concentrations

How much sugar (mol) is contained in a modest sip (~10 mL) of the soft drink from Example 2.2.2.1?

Solution

In this case, we can rearrange the definition of molarity to isolate the quantity sought, moles of sugar. We then substitute the value for molarity that we derived in Example 3.4.2, 0.375 M:

$$\begin{aligned} M &= \frac{\text{mol solute}}{\text{L solution}} & (2.2.2.2) \\ \text{mol solute} &= M \times \text{L solution} \\ \text{mol solute} &= 0.375 \frac{\text{mol sugar}}{\text{L}} \times \left(10 \text{ mL} \times \frac{1 \text{ L}}{1000 \text{ mL}} \right) = 0.004 \text{ mol sugar} \end{aligned}$$

? Exercise 2.2.2.2

What volume (mL) of the sweetened tea described in Example 2.2.2.1 contains the same amount of sugar (mol) as 10 mL of the soft drink in this example?

Answer

80 mL

✓ Example 2.2.2.3: Calculating Molar Concentrations from the Mass of Solute

Distilled white vinegar (Figure 2.2.2.2) is a solution of acetic acid, $\text{CH}_3\text{CO}_2\text{H}$, in water. A 0.500-L vinegar solution contains 25.2 g of acetic acid. What is the concentration of the acetic acid solution in units of molarity?



Figure 2.2.2.3: Distilled white vinegar is a solution of acetic acid in water.

A label on a container is shown. The label has a picture of a salad with the words “Distilled White Vinegar,” and, “Reduced with water to 5% acidity,” written above it.

Solution

As in previous examples, the definition of molarity is the primary equation used to calculate the quantity sought. In this case, the mass of solute is provided instead of its molar amount, so we must use the solute’s molar mass to obtain the amount of solute in moles:

$$M = \frac{\text{mol solute}}{\text{L solution}} = \frac{25.2 \text{ g CH}_3\text{CO}_2\text{H} \times \frac{1 \text{ mol CH}_3\text{CO}_2\text{H}}{60.052 \text{ g CH}_3\text{CO}_2\text{H}}}{0.500 \text{ L solution}} = 0.839 \text{ M} \quad (2.2.2.3)$$

$$M = \frac{0.839 \text{ mol solute}}{1.00 \text{ L solution}}$$

Nov 29, 2019, 5:24 PM

$$M = \frac{\text{mol solute}}{\text{L solution}} = 0.839 \text{ M} \quad (2.2.2.4)$$

? Exercise 2.2.2.3

Calculate the molarity of 6.52 g of CoCl_2 (128.9 g/mol) dissolved in an aqueous solution with a total volume of 75.0 mL.

Answer

0.674 M

✓ Example 2.2.2.4: Determining the Mass of Solute in a Given Volume of Solution

How many grams of NaCl are contained in 0.250 L of a 5.30-M solution?

Solution

The volume and molarity of the solution are specified, so the amount (mol) of solute is easily computed as demonstrated in Example 2.2.2.3

$$M = \frac{\text{mol solute}}{\text{L solution}} \quad (2.2.2.5)$$

$$\text{mol solute} = M \times \text{L solution} \quad (2.2.2.6)$$

$$\text{mol solute} = 5.30 \frac{\text{mol NaCl}}{\text{L}} \times 0.250 \text{ L} = 1.325 \text{ mol NaCl} \quad (2.2.2.7)$$

Finally, this molar amount is used to derive the mass of NaCl:

$$1.325 \text{ mol NaCl} \times \frac{58.44 \text{ g NaCl}}{\text{mol NaCl}} = 77.4 \text{ g NaCl} \quad (2.2.2.8)$$

? Exercise 2.2.2.4

How many grams of CaCl_2 (110.98 g/mol) are contained in 250.0 mL of a 0.200-M solution of calcium chloride?

Answer

5.55 g CaCl_2

When performing calculations stepwise, as in Example 2.2.2.3 it is important to refrain from rounding any intermediate calculation results, which can lead to rounding errors in the final result. In Example 2.2.2.4 the molar amount of NaCl computed in the first step, 1.325 mol, would be properly rounded to 1.32 mol if it were to be reported; however, although the last digit (5) is not significant, it must be retained as a guard digit in the intermediate calculation. If we had not retained this guard digit, the final calculation for the mass of NaCl would have been 77.1 g, a difference of 0.3 g.

In addition to retaining a guard digit for intermediate calculations, we can also avoid rounding errors by performing computations in a single step (Example 2.2.2.5). This eliminates intermediate steps so that only the final result is rounded.

✓ Example 2.2.2.5: Determining the Volume of Solution

In Example 2.2.2.3 we found the typical concentration of vinegar to be 0.839 M. What volume of vinegar contains 75.6 g of acetic acid?

Solution

First, use the molar mass to calculate moles of acetic acid from the given mass:

$$\text{g solute} \times \frac{\text{mol solute}}{\text{g solute}} = \text{mol solute} \quad (2.2.2.9)$$

Then, use the molarity of the solution to calculate the volume of solution containing this molar amount of solute:

$$\text{mol solute} \times \frac{\text{L solution}}{\text{mol solute}} = \text{L solution} \quad (2.2.2.10)$$

Combining these two steps into one yields:

$$\text{g solute} \times \frac{\text{mol solute}}{\text{g solute}} \times \frac{\text{L solution}}{\text{mol solute}} = \text{L solution} \quad (2.2.2.11)$$

$$75.6 \text{ g CH}_3\text{CO}_2\text{H} \left(\frac{\text{mol CH}_3\text{CO}_2\text{H}}{60.05 \text{ g}} \right) \left(\frac{\text{L solution}}{0.839 \text{ mol CH}_3\text{CO}_2\text{H}} \right) = 1.50 \text{ L solution} \quad (2.2.2.12)$$

? Exercise 2.2.2.5:

What volume of a 1.50-M KBr solution contains 66.0 g KBr?

Answer

0.370 L

Dilution of Solutions

Dilution is the process whereby the concentration of a solution is lessened by the addition of solvent. For example, we might say that a glass of iced tea becomes increasingly diluted as the ice melts. The water from the melting ice increases the volume of the

solvent (water) and the overall volume of the solution (iced tea), thereby reducing the relative concentrations of the solutes that give the beverage its taste (Figure 2.2.2.2).

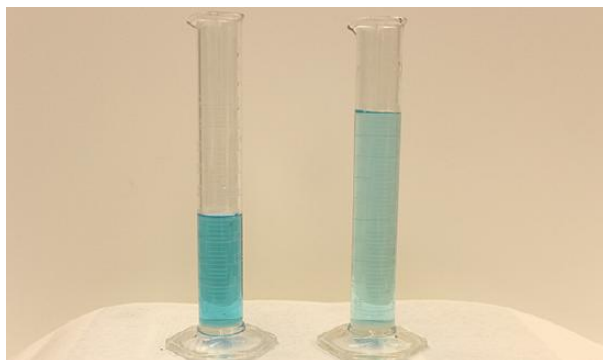


Figure 2.2.2.2: Both solutions contain the same mass of copper nitrate. The solution on the right is more dilute because the copper nitrate is dissolved in more solvent. (credit: Mark Ott).

This figure shows two graduated cylinders side-by-side. The first has about half as much blue liquid as the second. The blue liquid is darker in the first cylinder than in the second.

Dilution is also a common means of preparing solutions of a desired concentration. By adding solvent to a measured portion of a more concentrated *stock solution*, we can achieve a particular concentration. For example, commercial pesticides are typically sold as solutions in which the active ingredients are far more concentrated than is appropriate for their application. Before they can be used on crops, the pesticides must be diluted. This is also a very common practice for the preparation of a number of common laboratory reagents (Figure 2.2.2.3).



Figure 2.2.2.3: A solution of $KMnO_4$ is prepared by mixing water with 4.74 g of $KMnO_4$ in a flask. (credit: modification of work by Mark Ott)

This figure shows two photos. In the first, there is an empty glass container, 4.75 g of $KMnO_4$ powder on a white circle, and a bottle of distilled water. In the second photo the powder and about half the water have been added to the glass container. The liquid in the glass container is almost black in color.

A simple mathematical relationship can be used to relate the volumes and concentrations of a solution before and after the dilution process. According to the definition of molarity, the molar amount of solute in a solution is equal to the product of the solution's molarity and its volume in liters:

$$n = ML$$

Expressions like these may be written for a solution before and after it is diluted:

$$n_1 = M_1 L_1$$

$$n_2 = M_2 L_2$$

where the subscripts "1" and "2" refer to the solution before and after the dilution, respectively. Since the dilution process *does not change the amount of solute in the solution*, $n_1 = n_2$. Thus, these two equations may be set equal to one another:

$$M_1 L_1 = M_2 L_2$$

This relation is commonly referred to as the dilution equation. Although we derived this equation using molarity as the unit of concentration and liters as the unit of volume, other units of concentration and volume may be used, so long as the units properly cancel per the factor-label method. Reflecting this versatility, the dilution equation is often written in the more general form:

$$C_1 V_1 = C_2 V_2$$

where C and V are concentration and volume, respectively.

✓ Example 2.2.2.6: Determining the Concentration of a Diluted Solution

If 0.850 L of a 5.00-M solution of copper nitrate, $\text{Cu}(\text{NO}_3)_2$, is diluted to a volume of 1.80 L by the addition of water, what is the molarity of the diluted solution?

Solution

We are given the volume and concentration of a stock solution, V_1 and C_1 , and the volume of the resultant diluted solution, V_2 . We need to find the concentration of the diluted solution, C_2 . We thus rearrange the dilution equation in order to isolate C_2 :

$$C_1 V_1 = C_2 V_2$$
$$C_2 = \frac{C_1 V_1}{V_2}$$

Since the stock solution is being diluted by more than two-fold (volume is increased from 0.85 L to 1.80 L), we would expect the diluted solution's concentration to be less than one-half 5 M. We will compare this ballpark estimate to the calculated result to check for any gross errors in computation (for example, such as an improper substitution of the given quantities). Substituting the given values for the terms on the right side of this equation yields:

$$C_2 = \frac{0.850 \text{ L} \times 5.00 \frac{\text{mol}}{\text{L}}}{1.80 \text{ L}} = 2.36 \text{ M}$$

This result compares well to our ballpark estimate (it's a bit less than one-half the stock concentration, 5 M).

? Exercise 2.2.2.6

What is the concentration of the solution that results from diluting 25.0 mL of a 2.04-M solution of CH_3OH to 500.0 mL?

Answer

0.102 M CH_3OH

✓ Example 2.2.2.7: Volume of a Diluted Solution

What volume of 0.12 M HBr can be prepared from 11 mL (0.011 L) of 0.45 M HBr?

Solution

We are given the volume and concentration of a stock solution, V_1 and C_1 , and the concentration of the resultant diluted solution, C_2 . We need to find the volume of the diluted solution, V_2 . We thus rearrange the dilution equation in order to isolate V_2 :

$$C_1 V_1 = C_2 V_2$$
$$V_2 = \frac{C_1 V_1}{C_2}$$

Since the diluted concentration (0.12 M) is slightly more than one-fourth the original concentration (0.45 M), we would expect the volume of the diluted solution to be roughly four times the original volume, or around 44 mL. Substituting the given values and solving for the unknown volume yields:

$$V_2 = \frac{(0.45 \text{ M})(0.011 \text{ L})}{(0.12 \text{ M})}$$

$$V_2 = 0.041 \text{ L}$$

The volume of the 0.12-M solution is 0.041 L (41 mL). The result is reasonable and compares well with our rough estimate.

? Exercise 2.2.2.7

A laboratory experiment calls for 0.125 M HNO_3 . What volume of 0.125 M HNO_3 can be prepared from 0.250 L of 1.88 M HNO_3 ?

Answer

3.76 L

✓ Example 2.2.2.8: Volume of a Concentrated Solution Needed for Dilution

What volume of 1.59 M KOH is required to prepare 5.00 L of 0.100 M KOH?

Solution

We are given the concentration of a stock solution, C_1 , and the volume and concentration of the resultant diluted solution, V_2 and C_2 . We need to find the volume of the stock solution, V_1 . We thus rearrange the dilution equation in order to isolate V_1 :

$$C_1 V_1 = C_2 V_2$$

$$V_1 = \frac{C_2 V_2}{C_1}$$

Since the concentration of the diluted solution 0.100 M is roughly one-sixteenth that of the stock solution (1.59 M), we would expect the volume of the stock solution to be about one-sixteenth that of the diluted solution, or around 0.3 liters. Substituting the given values and solving for the unknown volume yields:

$$V_1 = \frac{(0.100 \text{ M})(5.00 \text{ L})}{1.59 \text{ M}}$$

$$V_1 = 0.314 \text{ L}$$

Thus, we would need 0.314 L of the 1.59-M solution to prepare the desired solution. This result is consistent with our rough estimate.

? Exercise 2.2.2.8

What volume of a 0.575-M solution of glucose, $\text{C}_6\text{H}_{12}\text{O}_6$, can be prepared from 50.00 mL of a 3.00-M glucose solution?

Answer

0.261

Summary

Solutions are homogeneous mixtures. Many solutions contain one component, called the solvent, in which other components, called solutes, are dissolved. An aqueous solution is one for which the solvent is water. The concentration of a solution is a measure of the relative amount of solute in a given amount of solution. Concentrations may be measured using various units, with one very useful unit being molarity, defined as the number of moles of solute per liter of solution. The solute concentration of a solution may be decreased by adding solvent, a process referred to as dilution. The dilution equation is a simple relation between concentrations and volumes of a solution before and after dilution.

Key Equations

- $M = \frac{\text{mol solute}}{\text{L solution}}$
- $C_1V_1 = C_2V_2$

Glossary

aqueous solution

solution for which water is the solvent

concentrated

qualitative term for a solution containing solute at a relatively high concentration

concentration

quantitative measure of the relative amounts of solute and solvent present in a solution

dilute

qualitative term for a solution containing solute at a relatively low concentration

dilution

process of adding solvent to a solution in order to lower the concentration of solutes

dissolved

describes the process by which solute components are dispersed in a solvent

molarity (M)

unit of concentration, defined as the number of moles of solute dissolved in 1 liter of solution

solute

solution component present in a concentration less than that of the solvent

solvent

solution component present in a concentration that is higher relative to other components

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2.2.3: Other Units for Solution Concentrations

Learning Objectives

- Define the concentration units of mass percentage, volume percentage, mass-volume percentage, parts-per-million (ppm), and parts-per-billion (ppb)
- Perform computations relating a solution's concentration and its components' volumes and/or masses using these units

In the previous section, we introduced molarity, a very useful measurement unit for evaluating the concentration of solutions. However, molarity is only one measure of concentration. In this section, we will introduce some other units of concentration that are commonly used in various applications, either for convenience or by convention.

Mass Percentage

Earlier in this chapter, we introduced percent composition as a measure of the relative amount of a given element in a compound. Percentages are also commonly used to express the composition of mixtures, including solutions. The mass percentage of a solution component is defined as the ratio of the component's mass to the solution's mass, expressed as a percentage:

$$\text{mass percentage} = \frac{\text{mass of component}}{\text{mass of solution}} \times 100\% \quad (2.2.3.1)$$

We are generally most interested in the mass percentages of solutes, but it is also possible to compute the mass percentage of solvent.

Mass percentage is also referred to by similar names such as *percent mass*, *percent weight*, *weight/weight percent*, and other variations on this theme. The most common symbol for mass percentage is simply the percent sign, %, although more detailed symbols are often used including %mass, %weight, and (w/w)%. Use of these more detailed symbols can prevent confusion of mass percentages with other types of percentages, such as volume percentages (to be discussed later in this section).

Mass percentages are popular concentration units for consumer products. The label of a typical liquid bleach bottle (Figure 2.2.3.1) cites the concentration of its active ingredient, sodium hypochlorite (NaOCl), as being 7.4%. A 100.0-g sample of bleach would therefore contain 7.4 g of NaOCl.



Figure 2.2.3.1: Liquid bleach is an aqueous solution of sodium hypochlorite (NaOCl). This brand has a concentration of 7.4% NaOCl by mass.

The sides of two cylindrical containers are shown. Each container's label is partially visible. The left container's label reads "Bleach." The right label contains more information about the product including the phrase, "Contains: Sodium hypochlorite 7.4%."

✓ Example 2.2.3.1: Calculation of Percent by Mass

A 5.0-g sample of spinal fluid contains 3.75 mg (0.00375 g) of glucose. What is the percent by mass of glucose in spinal fluid?

Solution

The spinal fluid sample contains roughly 4 mg of glucose in 5000 mg of fluid, so the mass fraction of glucose should be a bit less than one part in 1000, or about 0.1%. Substituting the given masses into the equation defining mass percentage yields:

$$\% \text{ glucose} = \frac{3.75 \text{ mg glucose} \times \frac{1 \text{ g}}{1000 \text{ mg}}}{5.0 \text{ g spinal fluid}} = 0.075\%$$

The computed mass percentage agrees with our rough estimate (it's a bit less than 0.1%).

Note that while any mass unit may be used to compute a mass percentage (mg, g, kg, oz, and so on), the same unit must be used for both the solute and the solution so that the mass units cancel, yielding a dimensionless ratio. In this case, we converted the units of solute in the numerator from mg to g to match the units in the denominator. We could just as easily have converted the denominator from g to mg instead. As long as identical mass units are used for both solute and solution, the computed mass percentage will be correct.

? Exercise 2.2.3.1

A bottle of a tile cleanser contains 135 g of HCl and 775 g of water. What is the percent by mass of HCl in this cleanser?

Answer

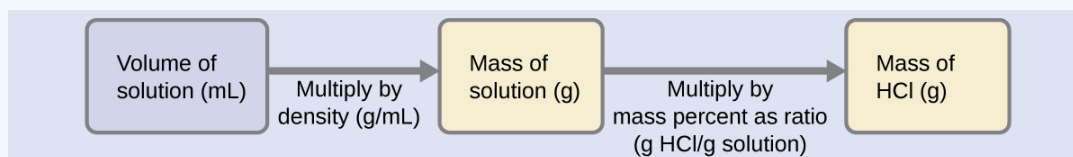
14.8%

✓ Example 2.2.3.2: Calculations using Mass Percentage

“Concentrated” hydrochloric acid is an aqueous solution of 37.2% HCl that is commonly used as a laboratory reagent. The density of this solution is 1.19 g/mL. What mass of HCl is contained in 0.500 L of this solution?

Solution

The HCl concentration is near 40%, so a 100-g portion of this solution would contain about 40 g of HCl. Since the solution density isn't greatly different from that of water (1 g/mL), a reasonable estimate of the HCl mass in 500 g (0.5 L) of the solution is about five times greater than that in a 100 g portion, or $5 \times 40 = 200$ g. To derive the mass of solute in a solution from its mass percentage, we need to know the corresponding mass of the solution. Using the solution density given, we can convert the solution's volume to mass, and then use the given mass percentage to calculate the solute mass. This mathematical approach is outlined in this flowchart:



A diagram of three boxes connected by a right-facing arrow in between each is shown. The box on the left contains the phrase, “Volume of solution (m L),” the middle box reads, “Mass of solution (g),” while the one on the right contains the phrase, “Mass of H C l (g).” There is a phrase under the left arrow that says, “Multiply by density (g / m L)” and under the right arrow it states, “Multiply by mass percent as ratio (g H C l / g solution).”

For proper unit cancellation, the 0.500-L volume is converted into 500 mL, and the mass percentage is expressed as a ratio, 37.2 g HCl/g solution:

$$500 \text{ mL solution} \left(\frac{1.19 \text{ g solution}}{\text{mL solution}} \right) \left(\frac{37.2 \text{ g HCl}}{100 \text{ g solution}} \right) = 221 \text{ g HCl}$$

This mass of HCl is consistent with our rough estimate of approximately 200 g.

? Exercise 2.2.3.2

What volume of concentrated HCl solution contains 125 g of HCl?

Answer

282 mL

Volume Percentage

Liquid volumes over a wide range of magnitudes are conveniently measured using common and relatively inexpensive laboratory equipment. The concentration of a solution formed by dissolving a liquid solute in a liquid solvent is therefore often expressed as a volume percentage, %vol or (v/v)%:

$$\text{volume percentage} = \frac{\text{volume solute}}{\text{volume solution}} \times 100\% \quad (2.2.3.2)$$

✓ Example 2.2.3.3: Calculations using Volume Percentage

Rubbing alcohol (isopropanol) is usually sold as a 70%vol aqueous solution. If the density of isopropyl alcohol is 0.785 g/mL, how many grams of isopropyl alcohol are present in a 355 mL bottle of rubbing alcohol?

Solution

Per the definition of volume percentage, the isopropanol volume is 70% of the total solution volume. Multiplying the isopropanol volume by its density yields the requested mass:

$$355 \text{ mL solution} \left(\frac{70 \text{ mL isopropyl alcohol}}{100 \text{ mL solution}} \right) \left(\frac{0.785 \text{ g isopropyl alcohol}}{1 \text{ mL isopropyl alcohol}} \right) = 195 \text{ g isopropyl alcohol}$$

? Exercise 2.2.3.3

Wine is approximately 12% ethanol ($\text{CH}_3\text{CH}_2\text{OH}$) by volume. Ethanol has a molar mass of 46.06 g/mol and a density 0.789 g/mL. How many moles of ethanol are present in a 750-mL bottle of wine?

Answer

1.5 mol ethanol

Mass-Volume Percentage

“Mixed” percentage units, derived from the mass of solute and the volume of solution, are popular for certain biochemical and medical applications. A mass-volume percent is a ratio of a solute’s mass to the solution’s volume expressed as a percentage. The specific units used for solute mass and solution volume may vary, depending on the solution. For example, physiological saline solution, used to prepare intravenous fluids, has a concentration of 0.9% mass/volume (m/v), indicating that the composition is 0.9 g of solute per 100 mL of solution. The concentration of glucose in blood (commonly referred to as “blood sugar”) is also typically expressed in terms of a mass-volume ratio. Though not expressed explicitly as a percentage, its concentration is usually given in milligrams of glucose per deciliter (100 mL) of blood (Figure 2.2.3.2).

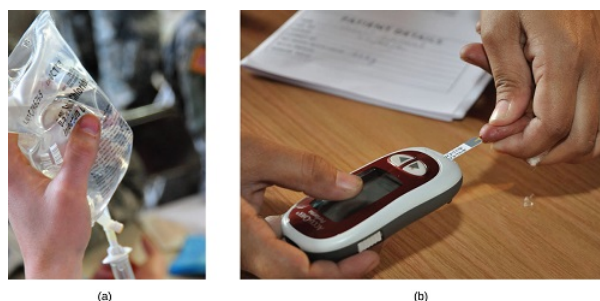


Figure 2.2.3.2: “Mixed” mass-volume units are commonly encountered in medical settings. (a) The NaCl concentration of physiological saline is 0.9% (m/v). (b) This device measures glucose levels in a sample of blood. The normal range for glucose concentration in blood (fasting) is around 70–100 mg/dL. (credit a: modification of work by “The National Guard”/Flickr; credit b: modification of work by Biswarup Ganguly).

Two pictures are shown labeled a and b. Picture a depicts a clear, colorless solution in a plastic bag being held in a person’s hand. Picture b shows a person’s hand holding a detection meter with a digital readout screen while another hand holds someone’s finger up to the end of the meter. The meter is pressed to the drop of blood that is at the end of the person’s finger.

Parts per Million and Parts per Billion

Very low solute concentrations are often expressed using appropriately small units such as parts per million (ppm) or parts per billion (ppb). Like percentage (“part per hundred”) units, ppm and ppb may be defined in terms of masses, volumes, or mixed mass-volume units. There are also ppm and ppb units defined with respect to numbers of atoms and molecules.

The mass-based definitions of ppm and ppb are given here:

$$\text{ppm} = \frac{\text{mass solute}}{\text{mass solution}} \times 10^6 \text{ ppm} \quad (2.2.3.3)$$

$$\text{ppb} = \frac{\text{mass solute}}{\text{mass solution}} \times 10^9 \text{ ppb} \quad (2.2.3.4)$$

Both ppm and ppb are convenient units for reporting the concentrations of pollutants and other trace contaminants in water. Concentrations of these contaminants are typically very low in treated and natural waters, and their levels cannot exceed relatively low concentration thresholds without causing adverse effects on health and wildlife. For example, the EPA has identified the maximum safe level of fluoride ion in tap water to be 4 ppm. Inline water filters are designed to reduce the concentration of fluoride and several other trace-level contaminants in tap water (Figure 2.2.3.3).

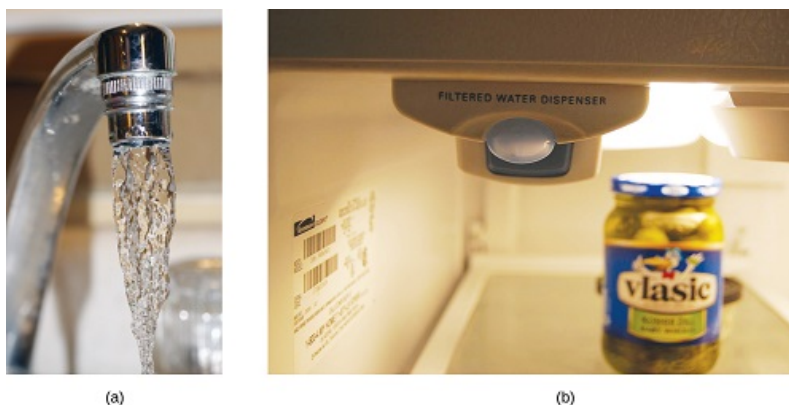


Figure 2.2.3.3: (a) In some areas, trace-level concentrations of contaminants can render unfiltered tap water unsafe for drinking and cooking. (b) Inline water filters reduce the concentration of solutes in tap water. (credit a: modification of work by Jenn Durfey; credit b: modification of work by “vastateparkstaff”/Wikimedia commons).

Two pictures are shown labeled a and b. Picture a depicts a clear, colorless solution in a plastic bag being held in a person’s hand. Picture b shows a person’s hand holding a detection meter with a digital readout screen while another hand holds someone’s finger up to the end of the meter. The meter is pressed to the drop of blood that is at the end of the person’s finger.

✓ Example 2.2.3.4: Parts per Million and Parts per Billion Concentrations

According to the EPA, when the concentration of lead in tap water reaches 15 ppb, certain remedial actions must be taken. What is this concentration in ppm? At this concentration, what mass of lead (μg) would be contained in a typical glass of water (300 mL)?

Solution

The definitions of the ppm and ppb units may be used to convert the given concentration from ppb to ppm. Comparing these two unit definitions shows that ppm is 1000 times greater than ppb ($1 \text{ ppm} = 10^3 \text{ ppb}$). Thus:

$$15 \text{ ppb} \times \frac{1 \text{ ppm}}{10^3 \text{ ppb}} = 0.015 \text{ ppm}$$

The definition of the ppb unit may be used to calculate the requested mass if the mass of the solution is provided. However, only the volume of solution (300 mL) is given, so we must use the density to derive the corresponding mass. We can assume the density of tap water to be roughly the same as that of pure water ($\sim 1.00 \text{ g/mL}$), since the concentrations of any dissolved substances should not be very large. Rearranging the equation defining the ppb unit and substituting the given quantities yields:

$$\text{ppb} = \frac{\text{mass solute}}{\text{mass solution}} \times 10^9 \text{ ppb}$$

$$\text{mass solute} = \frac{\text{ppb} \times \text{mass solution}}{10^9 \text{ ppb}}$$

$$\text{mass solute} = \frac{15 \text{ ppb} \times 300 \text{ mL} \times \frac{1.00 \text{ g}}{\text{mL}}}{10^9 \text{ ppb}} = 4.5 \times 10^{-6} \text{ g}$$

Finally, convert this mass to the requested unit of micrograms:

$$4.5 \times 10^{-6} \text{ g} \times \frac{1 \mu\text{g}}{10^{-6} \text{ g}} = 4.5 \mu\text{g}$$

? Exercise 2.2.3.4

A 50.0-g sample of industrial wastewater was determined to contain 0.48 mg of mercury. Express the mercury concentration of the wastewater in ppm and ppb units.

Answer

9.6 ppm, 9600 ppb

Summary

In addition to molarity, a number of other solution concentration units are used in various applications. Percentage concentrations based on the solution components' masses, volumes, or both are useful for expressing relatively high concentrations, whereas lower concentrations are conveniently expressed using ppm or ppb units. These units are popular in environmental, medical, and other fields where mole-based units such as molarity are not as commonly used.

Glossary

mass percentage

ratio of solute-to-solution mass expressed as a percentage

mass-volume percent

ratio of solute mass to solution volume, expressed as a percentage

parts per billion (ppb)

ratio of solute-to-solution mass multiplied by 10^9

parts per million (ppm)

ratio of solute-to-solution mass multiplied by 10^6

volume percentage

ratio of solute-to-solution volume expressed as a percentage

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2.3: Water Quality and Toxicity

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2.3.1: Chemical Contamination of Water

Learning Objectives

- Realize how combustion processes affect water sources.
- Define the pH and composition of acid rain (three specific formulas/names).
- Know the precursors of acid rain.
- Recall the environmental and biological effects of acid rain.
- Understand the differences between hard and soft water.
- Connect inorganic water contaminants with biological and environmental issues.
- Know the sources of inorganic and organic contaminants.
- Differentiate between organic and inorganic substances when given a formula.

The US Safe Drinking Water Act defines the term "contaminant" as meaning any physical, chemical, biological, or radiological substance or matter in water. Therefore, the "contaminant" definition very broadly applies as being anything other than water molecules. Drinking water may reasonably be expected to contain at least small amounts of some contaminants. Some drinking water contaminants may be harmful if consumed at certain levels in drinking water while others may be harmless. The presence of contaminants does not necessarily indicate that the water poses a health risk.

Air Pollutants

Water can become contaminated at any part of the water cycle. Air pollution can affect water vapor and water liquid. Combustion sources like vehicles and power plants generate compounds like NO_xs, SO_xs, CO, CO₂, and other various inorganic and organic volatile organic compounds (VOC) species. Some of these compounds can become soluble in water. This could affect pH (or acidity) level of water surface water. Rain water with a pH below 5.6 is considered to be acid rain.

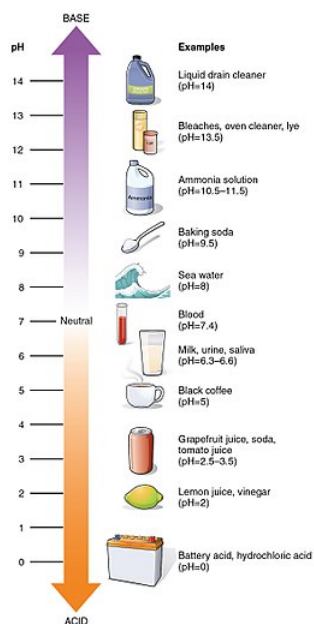


Figure 2.3.1.1: pH scale. (Copyright; OpenStax College via Anatomy & Physiology, Connexions Web site. <http://cnx.org/content/col11496/1.6/>)

Normally, the pH of water is a neutral value (or pH= 7). When NO_xs, SO_xs, CO, CO₂ enter the water cycle, then the pH level is lowered below 7.0. If these gases are absorbed in rain clouds, then acid rain results. Specific acids involved in acid rain are **sulfuric (H₂SO₄)**, **nitric (HNO₃)**, and **carbonic (H₂CO₃)**. This environmental problem affects living organisms and building materials. Acid solutions can corrode metals and make them soluble as well.

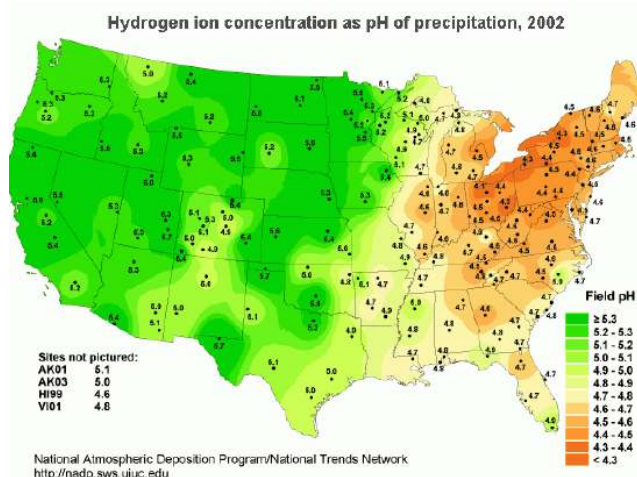
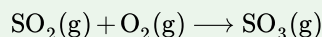


Figure 2.3.1.2: pH of rainwater over the continental United States.

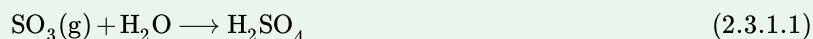
In the United States, the northeast has the most problems with acid rain. Concentrated populations that use electrical energy and vehicles contribute greatly to the pH reduction of rainwater. Reducing gaseous output requires capping combustion sources (vehicles and power plants). Acidity in rain is measured by collecting samples of rain and measuring its pH. To find the distribution of rain acidity, weather conditions are monitored and rain samples are collected at sites all over the country. The areas of greatest acidity (lowest pH values) are located in the Northeastern United States. This pattern of high acidity is caused by a large number of cities, the dense population, and the concentration of power and industrial plants in the Northeast. In addition, the prevailing wind direction brings storms and pollution to the Northeast from the Midwest, and dust from the soil and rocks in the Northeastern United States is less likely to neutralize acidity in the rain.

Acid rain from sulfuric acid

However, the majority of acid rain is accounted for by the presence of sulfuric acid (H_2SO_4).



Sulfur dioxide reacts with water to form sulfuric acid



Although sulfuric acid may be produced naturally in small quantities from biological decay and volcanic activity, it is produced almost entirely by human activity, especially the combustion of sulfur-containing fossil fuels in power plants.

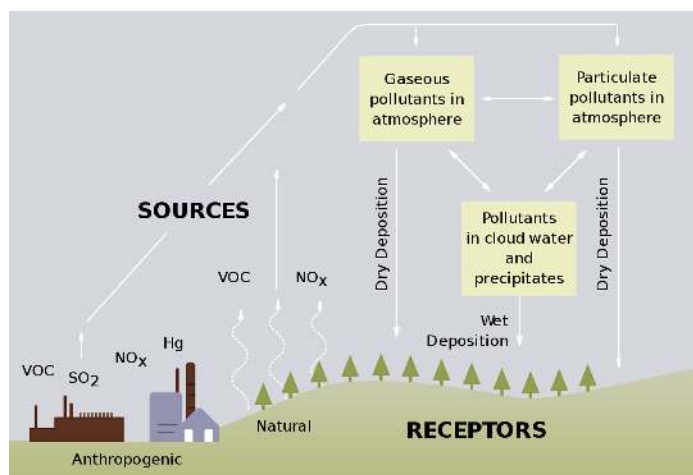
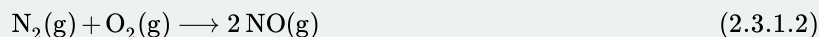


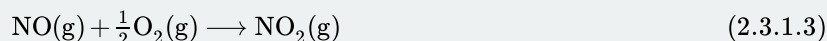
Figure 2.3.1.3: Processes involved in acid deposition (note that only SO_2 and NO_x play a significant role in acid rain). (public domain; EPA)

📌 Acid rain from nitric acid

Some of acid rain is accounted for by nitric acid (HNO_3) that originates from natural processes, but especially from high-temperature air combustion, such as occurs in car engines and power plants, that produces large amounts of NO gas. This gas then forms nitric acid via several steps. First nitric oxide (NO) is formed during lightning storms by the reaction of nitrogen and oxygen



and NO is oxidized to nitrogen dioxide (NO_2)



$\text{NO}_2(\text{g})$ then reacts with water droplets to generate nitric acid (HNO_3)

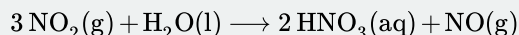


Table 2.3.1.2: Source of Water contamination in the United States

Combustion products	Sources
CO_2 and CO	Combustion of any material (any fuel or tree)
NO_x (NO_2 and NO)	High-temperature combustion of any fuel (gas, diesel, or coal), a product of lightning
SO_x (SO_2 and SO_3)	Combustion of sulfur-based fuels (diesel and coal), volcanic release
VOC (volatile organic compound)	Combustion of any carbon-based fuel (gas, diesel, or coal), fumes from paints or solvents

Inorganic Contaminants

Solubility of these species can be determined by consulting a solubility table (e.g., Table 4.7.1). These chemicals might be naturally present in a water source. Industry and agriculture also use and dispose of these types of chemicals as well. In determining the source of any pollutant, it is helpful to know a region's geology and proximity to chemical consumers. In this section, we will focus on a few inorganic species that can affect drinking water quality.

Hard Water

When water is described as being hard, then this means it has a large concentration of minerals. The **ions** that contribute to this problem are **calcium** (Ca^{2+}), **magnesium** (Mg^{2+}), **carbonate** (CO_3^{2-}), and **iron** ($\text{Fe}^{2+}/\text{Fe}^{3+}$). Hard water is not toxic, but can affect industrial processes. These ions will bond together to form insoluble salts that are called precipitates. Building up of these newly formed solids is called scale. Precipitates can collect in boilers, cooling towers, and any equipment that employs water. This buildup can affect how the equipment works by damaging it internally.

📌 Video: Hard Water

Watch this video below to get an idea of what hard water is.



<https://youtu.be/Ts6PNYk7-a0>

1. What chemical species cause hard water?
2. How does hard water affect industry?
3. Hard water is known to contribute to the formation of kidney stones. How else can this type of water affect the body?

Soft Water

Soft water does not contain an excessive amount of alkaline minerals. Instead, **potassium** (K^+) and **sodium** (Na^+) ions are present. Soft water does not form scale but does produce excessive lathers with soap. Although industry and consumers prefer soft water, the sodium content can affect health if ingested at a high concentration.

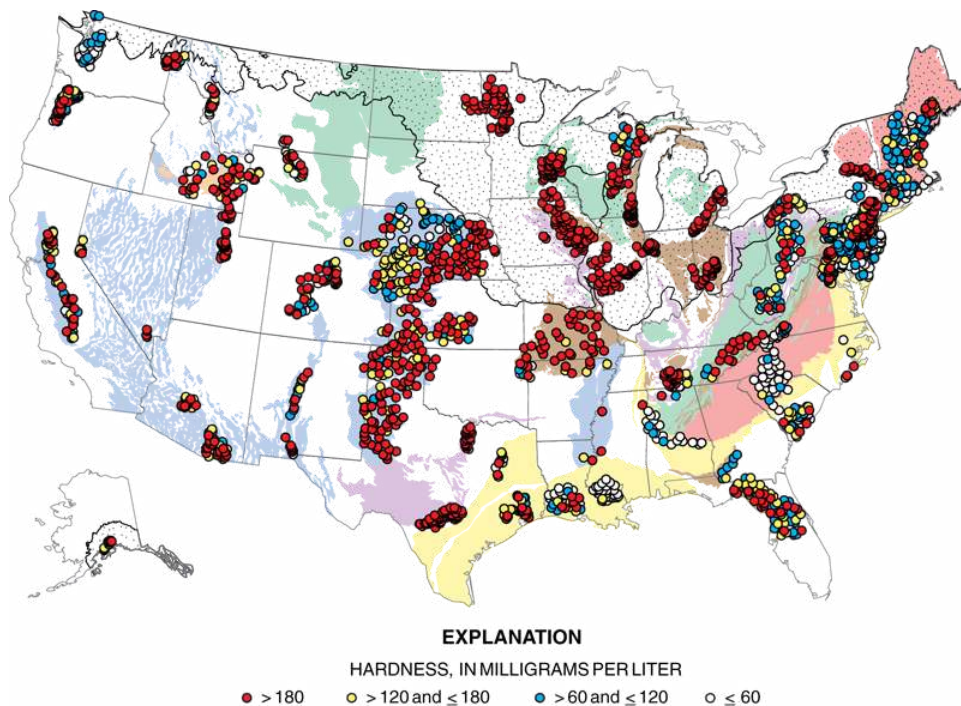


Figure 2.3.1.4: Hardness of groundwater from domestic wells, a USGS study. A study from the National Water-Quality Assessment (NAWQA) Program assessed water-quality conditions for about 2,100 domestic wells across the United States. (Public Domain; [USGS](#)).

Eutrophication

When pollutants enter a water system they originate from either point or non-point sources. If a single identifiable source can be located, then the pollutant originated from a point source. In contrast, non point sources indirectly contaminant water, air, or soil. Examples of non-point sources would be run-off and acid rain. Obviously, non-point pollutants are more difficult to regulate.

In agriculture, nitrates (NO_3^-) are used as fertilizers. Farmers can choose to use synthetic or natural (manure) nitrates. Regulating concentrations of these species could be difficult if all sources are not investigated and monitored. An excessive amount of these substances leads to [eutrophication](#). Many nitrate (NO_3^-) and phosphate (PO_4^{3-}) containing compounds are soluble in water. Once dissolved, these substances can travel to lakes and ponds. Here, these chemicals activate plants and algae to grow. Overgrowth of plant-life in water can inhibit oxygen from entering the water. As a result, aquatic animals are more likely to die in this environment. In addition, decomposition of organic material (once living) will be slow and smelly.



Figure 2.3.1.5: Algal bloom in village river. Taken in a small village in mountains near Chengdu, Sichuan, China. (CC BY-SA 3.0; [River algae Sichuan - Trophic state index - Wikipedia](#))

Eutrophication can be halted if phosphate (PO_4^{3-}) contamination is controlled. This involves limiting the use of some fertilizers and removing phosphates from detergents. Reducing nitrates can be a more challenging task. All compounds containing this polyatomic ion are extremely soluble. Moreover, controlling nitrate concentration from fecal material can be difficult.



Toxic Inorganic Species

Some inorganic compounds are quite soluble in water. If an aquatic system is acid, then solubility of these types of species can change. Lead and mercury based compounds are not as soluble as those in group IA of the periodic table. When the pH of water becomes acid, many of these once insoluble compounds now become dissolved and visually undetectable.

Lead (Action Level is 0.015 ppm)

Occupational exposure to lead is one of the most prevalent overexposures. Industries with high potential exposures include construction work, most smelter operations, radiator repair shops, and firing ranges. Other sources of lead based compounds include house paint (from before 1978), toys (older than 1976 or from abroad), pipes, faucets, jewelry, wet batteries (gasoline engine based), pottery, and Kohl/Kajol eyeliners.

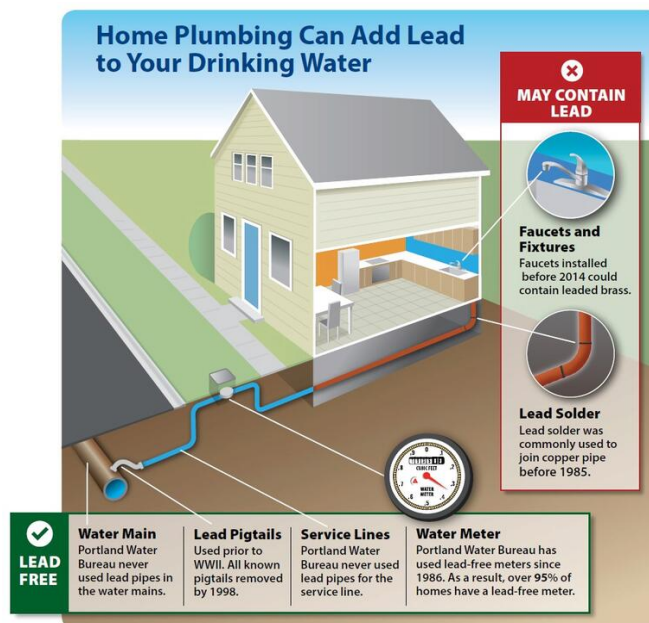


Figure 2.3.1.6: Lead and drinking water. (Copyright; City of Portland)

Gasoline products may contain lead compounds to diminish knocking of a combustion engine. These additives increase the octane level of a fuel which enables the engine to burn more effectively. Unfortunately, releasing lead-based fumes can impair a person's nervous system. In addition, other disorders and diseases (kidney issues, gastrointestinal problems, growth delays, anemia, and learning difficulties) will become more prevalent in an area that has signification combustion of lead based fuels. Children will be more impacted by lead poisoning than adults. Often, the damage done to this group of people is irreversible. By the early 1970's, the Environmental Protection Agency (EPA) started focusing on phasing out leaded fuel products. By the mid 1980's, most US vehicles used only unleaded fuels. The EPA banned lead based fuel in 1996. Today, only the aviation industry and off-road vehicles are allowed to use leaded fuel in the United States.

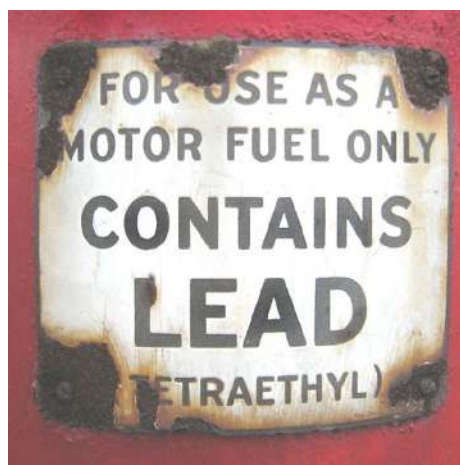


Figure 2.3.1.7: ead warning on a gas pump at Keeler's Korner, Lynnwood, Washington. Keeler's Korner, a former grocery store and gas station (built 1927) listed on the National Register of Historic Places, listed 1982, NRHP listing #82004287. (CC-BY-SA 3.0; <https://commons.wikimedia.org/wiki/User:Jmabel>)

Arsenic (0.010 ppm or 10 ppb)

Common sources of exposure to higher-than-average levels of arsenic include near or in hazardous waste sites and areas with high levels naturally occurring in soil, rocks, and water.

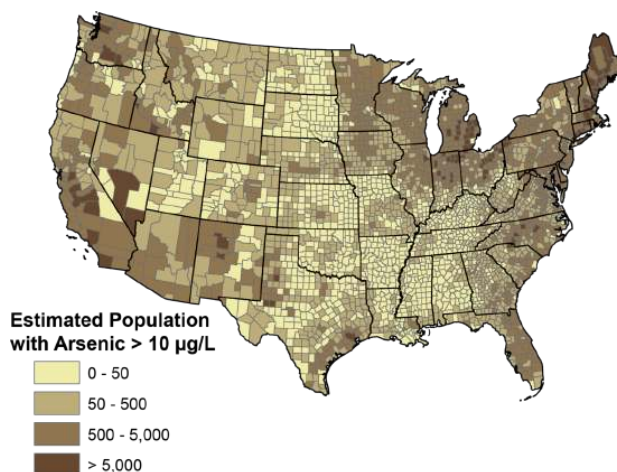


Figure 2.3.1.8: This map shows estimates of how many private domestic well users in each county may be drinking water with levels of arsenic of possible concern for human health. (µg/L, micrograms per liter) (USGS; [Arsenic and Drinking Water | U.S. Geological Survey \(usgs.gov\)](#))

Arsenic compounds can be found in lead/copper smelting processes, lumber pressurizing (copper chromated arsenate compounds are no longer used in the United States) and pesticide applications (organic arsenic compounds are used to treat cotton fields and orchards). Exposure to high levels of arsenic can cause skin lesions, neurological problems, gastrointestinal/liver illnesses, various cancers, and death.



Mercury (0.002 ppm)

Common sources of mercury exposure include mining, production, and transportation of mercury, as well as mining and refining of gold and silver ores. High mercury exposure results in permanent nervous system and kidney damage. Once inorganic mercury enters aquatic systems, it can transform into organic mercury or organometallic mercury. An example of one of these compounds is methyl mercury (CH_3Hg). This type of compound is quite toxic and has bioaccumulation effects.

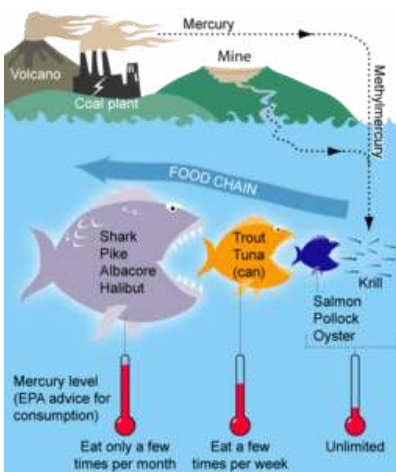


Figure 2.3.1.9: This figure shows some common sources of mercury, the conversion to toxic methylmercury and the outline of EPA consumption recommendations for certain types of fish based on mercury levels. (Copyright; Bretwood Higman, Ground Truth Trekking via <http://www.groundtruthtrekking.org/Graphics/Large/MercuryFoodChain-01.png>)

Cadmium (0.005 ppm)

Cadmium is an extremely toxic metal that exists naturally in the Earth's crust as a common. Agricultural crops absorb cadmium compounds from the soil. The average person is exposed to cadmium through the consumption of plant based food, burning of cadmium based materials (air pollution), and drinking of tap water. Tobacco consumers receive additional cadmium when they smoke. Lastly, artists might use cadmium based pigments for dramatic colors in their paintings.



Figure 2.3.1.10: The Berkeley Pit, an open pit copper mine in Butte, Montana. (Copyright; User:Cybergrl23 via Wikipedia Commons)

At industrial workplaces, cadmium can be introduced to the atmosphere when any metal ore is being processed or smelted. Some forms of steel and batteries (Ni-Cd) contain cadmium mixtures. Several deaths from acute exposure have occurred among welders who have unsuspectingly welded on cadmium-containing alloys or with silver solders. This chemical substance is carcinogenic and causes a signature painful bone disease. Lastly, cadmium exposure can cause significant damage to kidneys.

Uranium (30 ppb)

Natural deposits of this element are found in the earth crust are sometimes associated with mountainous regions of the world. In the United States, uranium ores can be found in the western part of the country. If uranium becomes soluble, then it can leach or move to other locations contaminating water and soil nearby.

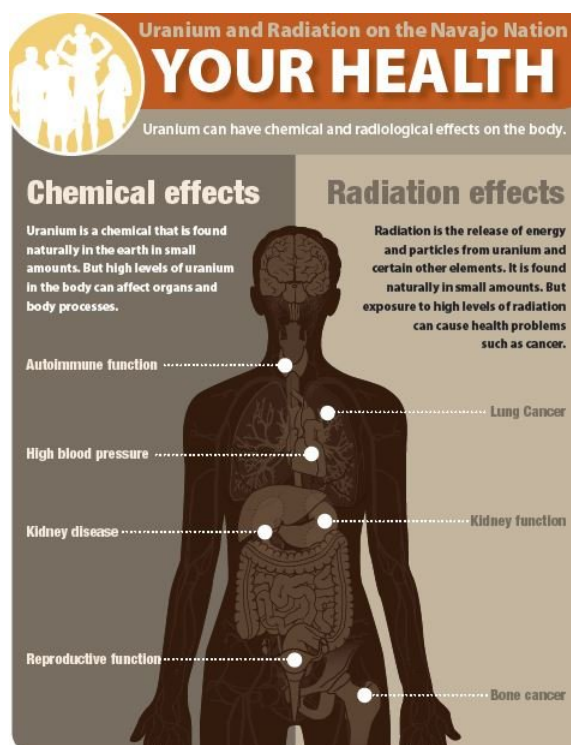


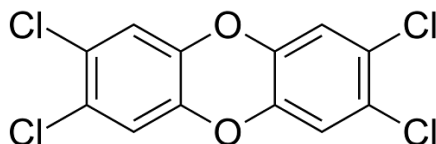
Figure 2.3.1.11: Your Health: Uranium and Radiation on the Navajo Nation. (epa.gov; [Health Effects of Uranium | US EPA](#))

Enriched U-235 (2-5%) is used for fuel in all US commercial nuclear power plants. Waste products of fuel use are stored for long periods of time above ground at most nuclear reactor facilities. Fuel waste can be stored in a wet or dry environment. Either method requires isolation from humans and the environment since the waste will be radioactive for a long time. Enriched U-235 (90%) was fuel for the Little Boy atomic bomb which was dropped over Hiroshima in 1945. At the time, purification of this form of uranium was difficult and costly. This resulted in the production of only one uranium type atomic weapon.

Organic Chemical Concerns

Dioxin (3.0×10^{-8} ppm)

Dioxins are mainly byproducts of industrial practices. They are produced through a variety of incineration processes, including improper municipal waste incineration and burning of trash, and can be released into the air during natural processes, such as forest fires and volcanoes. Dioxins are also produced in the bleaching process used by the paper industry. These chemicals have been classified as Persistent Organic Pollutants (POPs) because of their long residual life-times in the environment. These compounds are fat soluble and will accumulate in fatty tissues of living organisms which in turn affects the health of the food chain.



Dioxin based compounds harm hormonal and reproductive systems. In addition, immunity disorders and chloroacne can result if someone has been exposed to these types of chemicals. A famous case of intentional dioxin (TCDD) poisoning involved a former Ukrainian presidential candidate named Viktor Yushchenko. In 2004, environmental toxicologists in Austria detected extremely high concentrations of dioxins in Yushchenko's blood. Also, medical experiments noted the change in his complexion before and after the poisoning. For more information regarding this incident, please click [here](#).

When synthesizing Agent Orange (a herbicide used before and during the Vietnam War), chemists simultaneously and unintentionally produced dioxin. Exposure to this chemical derivative increased cancer rates to those exposed.



(PCB) Polychlorinated Biphenyls (5.0×10^{-4} ppm)

Once used as electrical insulators, the United States produced this family of compounds from the late 1930's through the 1970's. These compounds did not decompose, conduct electricity, and could withstand high temperature environments. For these reasons, PCBs were commonly incorporated into electrical transformers, fluorescent lights, capacitors and older household appliances (televisions and refrigerators).

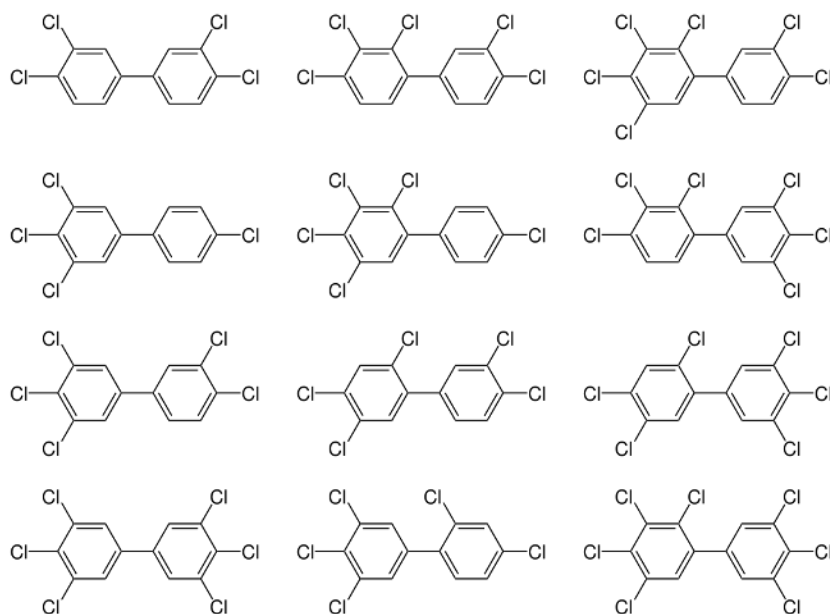


Figure 2.3.1.12: Structures of dioxin-like PCBs.. (Copyright; User:Leyo via Own work based on: M. Van den Berg et al. (2006). "The 2005 World Health Organization Reevaluation of Human and Mammalian Toxic Equivalency Factors for Dioxins and Dioxin-Like Compounds". *Toxicological Sciences* 93 (2): 223–241. DOI:10.1093/toxsci/kfl055. PMID 16829543.)

These compounds are classified as human carcinogens. In certain concentrations, PCB exposure can manifest as chloracne. Chronic exposure to PCBs can cause liver and central nervous system damage. Lastly, PCBs can cause reproductive issues as well.

<file:///C:/Users/egordon/Downloads/c...disaster-5.pdf>

References

1. ntp.niehs.nih.gov/ntp/roc/content/profiles/cadmium.pdf
2. [Lead Poisoning: Causes, Symptoms, and Diagnosis \(healthline.com\)](#)
3. [End Of Leaded Gasoline: World Has Stopped Using Toxic Additive : NPR](#)
4. [Arsenic | ToxFAQs™ | ATSDR \(cdc.gov\)](#)
5. [Learn about Dioxin | US EPA](#)

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2.3.2: Biological Contamination of Water

Learning Objectives

- Identify the three categories of pathogens that produce water-borne diseases.
- Provide one example of each pathogen, typical sources, and health problems.
- Summarize how water-borne diseases can be prevented and treated.
- Recall areas of the world where water is not properly sanitized.
- List foods and beverages that need to be avoided when using water that is not sanitized.
- Recall how long to boil water if under an advisory.
- Realize that boiling does not remove inorganics, metals, or organics.
- Besides boiling, discuss the chemical sanitation process of how to sanitize water at home (EPA method below).

Water Borne Diseases

If water is not cleaned properly, residents of a community can contract various illnesses. Viruses, bacteria, and parasites can enter a water supply unknowingly. All three of these species are pathogenic, or disease-causing. In the United States, the Environmental Protection Agency (EPA) quantifies and monitors these pathogens in water systems that serve at least 200 consumers. The EPA classifies these contaminants as being microorganisms (even though a biologist might dispute this terminology).



Video 2.3.2.1: The Coalition for Global Community Health is working within existing social structures in Belén, Iquitos, Peru to uphold the human rights of the community members. We speak directly with community members in an open forum to learn about their needs, desires, and ideas for creating an opportunity to change their communities for the better

Approximately 829,000 people die each year due to developing diarrheal illnesses from water based illnesses. Of the number, over 297,000 of these fatalities are children under five years of age. From a worldwide perspective, 785 million lack access to an improved water source. That is, this large group of people do not extract their water from a household connection, public standpipe, borehole/protected well, protected spring, or rainwater collection. Implementing water sanitation and hygiene for people who live in these countries could prevent at least 9.1% of the global disease burden and 6.3% of all deaths.



Figure 2.3.2.1: This young girl was collecting water from a sacred pond in Ogi, Nigeria, but she won't get Guinea worm because the water had been treated, and steps had been installed, so people couldn't contaminate the water. Creator: CDC/ The Carter Center. (Copyright, Public Health Library).

One of the many waterborne pathogens that can be contracted by drinking unclean water is **Giardiasis**. The picture below shows how a person might contract **Giardiasis** from *giardia*, a parasite. This particular pathogen can live in a body up to six months. Once detected through a stool sample, a patient can be prescribed specific antibiotics like Flagyl to treat the infection. Unfortunately, there is no vaccine for preventing Giardiasis.

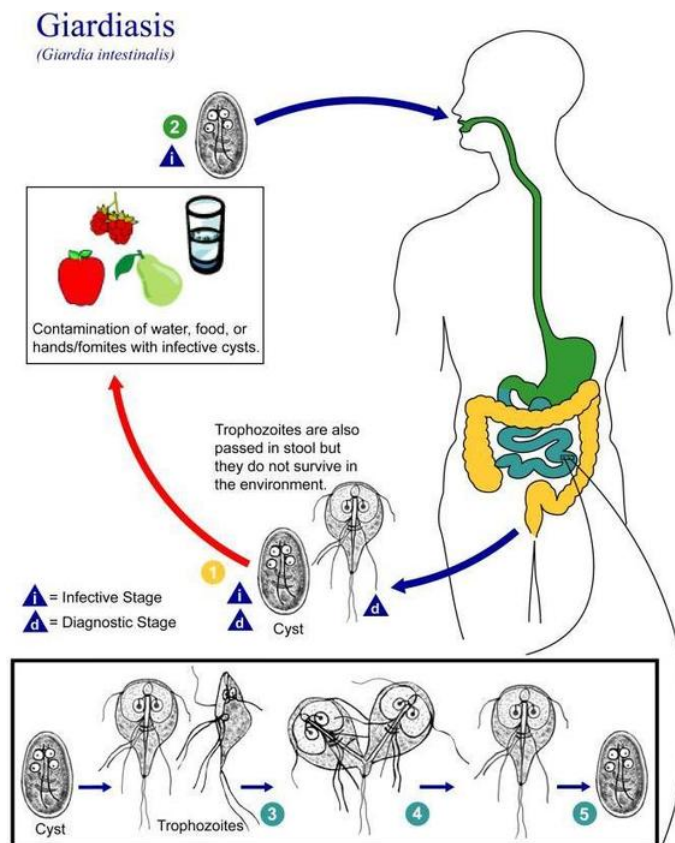


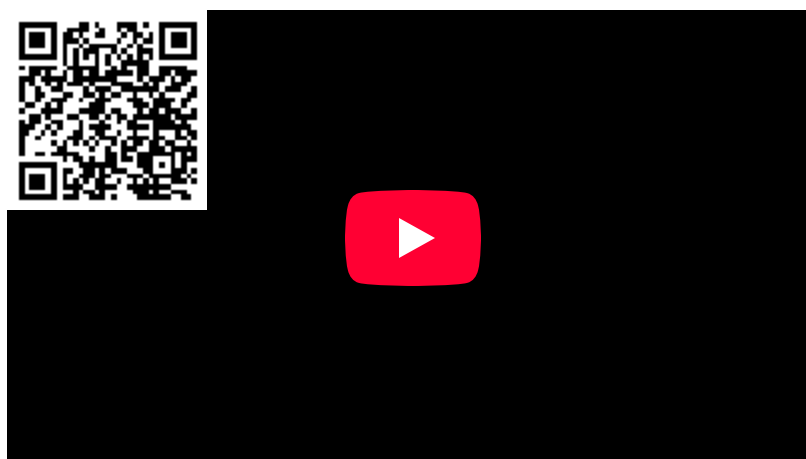
Figure 2.3.2.2: The life cycle of Giardia.

The table below shows water-borne diseases that can result from viruses, bacteria, and parasites. In some cases, vaccines are available. When eating, drinking, or swimming, it is important to be aware of how you could be affected by these pathogens. Sanitation of drinking water with chlorine-based compounds reduces the power of these pathogens. In addition, proper handling of foods and beverages could reduce your risk of developing one or more of the following health problems.

Table 2.3.2.1: Pathogens that cause waterborne illnesses.

Pathogen Name	Pathogen Type	Source	Health problem	Prevention/Treatment
<i>Giardia</i>	Parasite	Fecal contamination and uncooked food	Vomiting, diarrhea, and cramps	Medication afterward
<i>Cryptosporidium</i>	Parasite	Fecal contamination	Vomiting, diarrhea, fever, and cramps	Medication afterward
<i>Typhoid</i>	Bacteria	Fecal contamination	High fever, stomach pains, headache, and rash	Vaccination/Antibiotics
<i>E. coli</i>	Bacteria	Fecal contamination	Diarrhea and cramps	Fluids
<i>Legionella</i>	Bacteria	Found naturally in heated water	Causes Legionnaires (a type of pneumonia)	Medications afterward
<i>Cholera</i>	Bacteria	Related to fecal contamination or undercooked or raw shellfish	Diarrhea	Vaccine/Rehydration, antibiotics, and Zinc
<i>Hepatitis A</i>	Virus	Contaminated food and water	Vomiting, dark urine, and yellowing of the eyes.	Vaccination/Fluids
<i>Polio</i>	Virus	Fecal contamination	Flu symptoms, paralysis	Vaccination

When traveling to places that do not have comprehensive water sanitation procedures, it is important to avoid certain foods and beverages. Ice and tap water should be avoided to reduce risk of exposure to pathogens. In addition, vegetables and fruits that do not have a peel could cause water borne illness. If possible, purchase bottled water from a reputable company (Nestle is common in Asia and South America)



Center for Disease Control (CDC) Sanitizing Information

Water advisories may be declared if sanitation is compromised. In these situations, boiling, halogen disinfection, or filtration could be utilized to make water **potable** (drinkable). The Centers for Disease Control has developed a document to compare these different methods of sanitation. Look below to see the most effective ways to make water safe.

This document should only serve as a guide for individuals intending to use untreated or poorly treated water as a drinking water source. This document may also aid travelers and backcountry water users in researching drinking water treatment methods. Except for boiling, few of the water treatment methods are 100% effective in removing all pathogens.				Table Key for Pathogen Removal			
				-	not effective		
				+	low effectiveness		
				++	moderate effectiveness		
				+++	high effectiveness		
				++++	very high effectiveness		
Contaminant	Potential Health Effects from Ingestion of Water	Sources of Contaminant in Drinking Water	Methods that may remove some/all of the contaminant				
			REMEMBER: If boiling water is not a feasible option, the most effective pathogen reduction method in untreated or poorly treated drinking water is a combination treatment, using the appropriate filtration and disinfection methods.				
			Boiling (Rolling boil for 1 minute minimum) *	Filtration **	Disinfection***		Combination Filtration and Disinfection****
					Iodine or Chlorine	Chlorine Dioxide	
Protozoa- <i>Cryptosporidium</i>	Gastrointestinal illness (e.g., diarrhea, vomiting, cramps)	Human and animal fecal waste	++++	+++ Absolute ≤ 1.0 micron filter (NSF Standard 53 or 58 rated "cyst reduction / removal" filter)	-	+ to ++	++++ Absolute ≤ 1.0 micron filter (NSF Standard 53 or 58 rated "cyst reduction / removal" filter)
Protozoa- <i>Giardia intestinalis</i> (aka <i>Giardia lamblia</i>)	Gastrointestinal illness (e.g., diarrhea, vomiting, cramps)	Human and animal fecal waste	++++	+++ Absolute ≤ 1.0 micron filter (NSF Standard 53 or 58 rated "cyst reduction / removal" filter)	+ to ++	+++	++++ Absolute ≤ 1.0 micron filter (NSF Standard 53 or 58 rated "cyst reduction / removal" filter)
Bacteria- (e.g., <i>Campylobacter</i> , <i>Salmonella</i> , <i>Shigella</i> , <i>E. coli</i>)	Gastrointestinal illness (e.g., diarrhea, vomiting, cramps)	Human and animal fecal waste	++++	++ Absolute ≤ 0.3 micron filter	+++	+++	++++ Absolute ≤ 0.3 micron filter
Viruses- (e.g., enterovirus, hepatitis A, norovirus, rotavirus)	Gastrointestinal illness (e.g., diarrhea, vomiting, cramps)	Human and animal fecal waste	++++	-	+++	+++	+++
Treatment methods listed above:							
* Boiling can be used as a pathogen reduction method that should kill all pathogens. Water should be brought to a rolling boil for 1 minute (at altitudes greater than 6,562 feet (>2,000 m), boil water for 3 minutes.)							
** Filtration can be used as a pathogen reduction method against most microorganisms, depending on the pore size of the filter, amount of the contaminant, particle size of the contaminant, and charge of the contaminant particle. Manufacturer's instructions must be followed. More information on selecting an appropriate water filter can be found at www.cdc.gov/crypto/factsheets/filters.html . Only filters that contain a chemical disinfectant matrix will be effective against some viruses.							
*** Disinfection can be used as a pathogen reduction method against microorganisms. However, contact time, disinfectant concentration, water temperature, water turbidity (cloudiness), water pH, and many other factors can impact the effectiveness of chemical disinfection. The length of time and concentration of disinfectant varies by manufacturer and effectiveness of pathogen reduction depends on the product. Depending on these factors, 100% effectiveness may not be achieved. Manufacturer's instructions must be followed.							
**** If boiling water is not possible, a Combination of Filtration and Chemical Disinfection is the most effective pathogen reduction method in drinking water for backcountry or travel use. Manufacturer's instructions must be followed.							
Other treatment methods can be effective against some of the above pathogens:							
• Ultraviolet Light (UV Light) can be used as a pathogen reduction method against some microorganisms. The technology requires effective prefiltering due to its dependence on low water turbidity (cloudiness), the correct power delivery, and correct contact times to achieve maximum pathogen reduction. UV might be an effective method for pathogen reduction in untreated or poorly treated water; there is a lack of independent testing data available on specific systems. Manufacturer's instructions must be followed.							
• MIOX® systems use a salt solution to create mixed oxidants, primarily chlorine. As a result, refer to the category above for chlorine disinfection. Manufacturer's instructions must be followed.							
Important: Water that has been disinfected with iodine is NOT recommended for pregnant women, people with thyroid problems, those with known hypersensitivity to iodine, or continuous use for more than a few weeks at a time.							
In addition to using the appropriate drinking water treatment methods listed above, you can also protect yourself and others from waterborne illness by:							
• Burying human waste 8 inches deep and at least 200 feet away from natural waters.							
• Practicing good personal hygiene. Wash hands before handling food, eating, and after using the toilet.							

Halogen based solids can be purchased at most home improvement stores, pool stores, Walmart, and Target. These chemicals will alter taste and smell of water. These chemicals are also needed when properly sanitizing a pool or a hot tub. Halogen tablets are quite cheap and an effective way for sanitizing any type of water.

EPA: EMERGENCY DISINFECTION OF DRINKING WATER

In an emergency situation where regular water service has been interrupted – like a hurricane, flood, or water pipe breakage – local authorities may recommend using only bottled water, boiled water, or disinfected water until regular water service is restored. The instructions below show you how to boil and disinfect water to kill most disease-causing microorganisms that may be present in the water. However, boiling or disinfection will not destroy other contaminants, such as heavy metals, salts, and most other chemicals.

ONLY USE WATER THAT HAS BEEN PROPERLY DISINFECTED FOR DRINKING, COOKING, MAKING ANY PREPARED DRINK, WASHING DISHES, AND FOR BRUSHING TEETH.

Use **bottled water** or water you have properly prepared and stored as an emergency water supply.

Boil water, if you do not have bottled water. Boiling is sufficient to kill pathogenic bacteria, viruses and protozoa (WHO, 2015).

- If water is cloudy, let it settle and filter it through a clean cloth, paper towel, or coffee filter.

- Bring water to a rolling boil for at least one minute. At altitudes above 5,000 feet (1,000 meters), boil water for three minutes.
- Let the water cool naturally and store it in clean containers with covers.
- To improve the flat taste of boiled water, add one pinch of salt to each quart or liter of water, or pour the water from one clean container to another several times.

Disinfect water using household bleach, if you can't boil water. Only use regular, unscented chlorine bleach products that are suitable for disinfection and sanitization as indicated on the label. The label may say that the active ingredient contains 6 or 8.25% of sodium hypochlorite. Do not use scented, color safe, or bleaches with added cleaners.

- If water is cloudy, let it settle and filter it through a clean cloth, paper towel, or coffee filter.
- Locate a clean dropper from your medicine cabinet or emergency supply kit.
- Locate a fresh liquid chlorine bleach or liquid chlorine bleach that is stored at room temperatures for less than one year.
- Use the table on the next page as a guide to decide how much bleach you should add to the water, for example, add 8 drops of 6 % bleach or 6 drops of 8.25% bleach to each gallon of water. Double the amount of bleach if the water is cloudy, colored, or very cold.
- Stir and let stand for 30 minutes. The water should have a slight chlorine odor. If it doesn't, repeat the dosage and let stand for another 15 minutes before use.
- If the chlorine taste is too strong, pour the water from one clean container to another and let it stand for a few hours before use.

Volume of Water	Amount of 6% Bleach to Add [†]	Amount of 8.25% Bleach to Add [†]
1 quart/liter	2 drops	2 drops
1 gallon	8 drops	6 drops
2 gallons	16 drops (1/4 tsp.)	12 drops (1/4 tsp.)
4 gallons	1/3 tsp.	1/4 tsp.
8 gallons	2/3 tsp.	1/2 tsp.

[†]Bleach may contain 6 or 8.25% sodium hypochlorite

ADDITIONAL WATER GUIDANCE FOR EMERGENCIES

Prepare and store an emergency water supply. Visit the Federal Emergency Management Agency (FEMA) website for additional guidance on preparing and storing an emergency water supply.

Look for other sources of water in and around your home. Although bottled water is your best choice, you may be able to find other sources of water by melting ice cubes or draining your hot water tank or pipes. You can also use river or lake water. It is generally better to use flowing water than still, stagnant water. However, do not use water with floating material in it or water that has a dark color or questionable odor. Regardless of the source, treat the water by following the instructions above. If you have a well on your property that has been flooded, make sure to disinfect and test the well water after the flood. Contact your state or local health department for advice or go [here](#).

Consider how the water looks and how to filter it if needed. Disinfection does not work as well when water is cloudy or colored. If water is cloudy, let it settle. Then filter the water through a clean cloth, paper towel, or coffee filter. Store the settled and filtered water in clean containers with covers

OTHER DISINFECTION METHODS

If you don't have liquid bleach, you can use one of the other disinfection methods described below.

- *Granular calcium hypochlorite.* The first step is to make a chlorine solution that you will use to disinfect your water. For your safety, do it in a ventilated area and wear eye protection. Add one heaping teaspoon (approximately ¼ ounce) of high-test granular calcium hypochlorite (HTH) to two gallons of water and stir until the particles have dissolved. The mixture will produce a chlorine solution of approximately 500 milligrams per liter. To disinfect water, add one part of the chlorine solution to every 100 parts of water you are treating. This is about the same as adding 1 pint (16 ounces) of the chlorine solution to 12.5 gallons of water. If the chlorine taste is too strong, pour the water from one clean container to another and

let it stand for a few hours before use. CAUTION: HTH is a very powerful oxidant. Follow the instructions on the label for safe handling and storage of this chemical.

- *Common household iodine* (or “tincture of iodine”). You may have iodine in your medicine cabinet or first aid kit. Add five drops of 2% tincture of iodine to each quart or liter of water that you are disinfecting. If the water is cloudy or colored, add 10 drops of iodine. Stir and let the water stand for at least 30 minutes before use.
- *Water disinfection tablets*. You can disinfect water with tablets that contain chlorine, iodine, chlorine dioxide, or other disinfecting agents. These tablets are available online or at pharmacies and sporting goods stores. Follow the instructions on the product label as each product may have a different strength.

Safe Drinking Water Hotline: 1-800-426-4791 [water.epa.gov/drink/hotline](https://www.water.epa.gov/drink/hotline)

✓ Example 2.3.2.1

1. Do all waterborne pathogens cause stomach illnesses?
2. If your community is under a water advisory, then how long should you boil tap water to kill pathogens?
3. Vaccinations and preventive medications can protect you from which pathogens?
4. When properly diluted, which common household cleaner can sanitize tap water?

Answer

1. Legionella bacteria causes respiratory problems. Also, hepatitis and polio viruses do not produce stomach illnesses.
2. Water should be boiled rigorously for at least one minute to kill most pathogens.
3. Vaccines can be used to prevent: hepatitis, typhoid, cholera, and polio. In the United States, most children have been vaccinated from hepatitis and polio. When traveling to destinations that lack sanitized water, it would be beneficial to request prescription medications from your health care professional. Refer to the chart above regarding which diseases can be treated with medications.
4. A diluted (watered down) form of bleach (sodium hypochlorite) can be used to sanitize water. Please note the different types of bleach that can be purchased. In addition, do not use color safe or scented bleach.

References

1. World Health Organization. [Drinking-water \(who.int\)](https://www.who.int)
2. The Center For Disease Control. [Global WASH Fast Facts](#) | [Global Water, Sanitation and Hygiene](#) | [Healthy Water](#) | CDC

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2.4: Drug Dosing and Overdoses

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CHAPTER OVERVIEW

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3.4.2: Other Water treatment processes

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3.1: How do molecules interact?

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3.1.1: Prelude to Liquids and Solids

The great distances between atoms and molecules in a gaseous phase, and the corresponding absence of any significant interactions between them, allows for simple descriptions of many physical properties that are the same for all gases, regardless of their chemical identities. As described in the final module of the chapter on gases, this situation changes at high pressures and low temperatures—conditions that permit the atoms and molecules to interact to a much greater extent.



Figure 3.1.1.1: Solid carbon dioxide (“dry ice”, left) sublimates vigorously when placed in a liquid (right), cooling the liquid and generating a fog of condensed water vapor above the cylinder. (credit: modification of work by Paul Flowers)

This figure shows pieces of a white substance which appear to be sublimating. To the right of these pieces are three graduated cylinders. Each cylinder holds a different color liquid, and above the liquid, the cylinders are filled with a fog-like substance. This fog-like substance swirls out of the top and around the outside of the cylinders.

In the liquid and solid states, these interactions are of considerable strength and play an important role in determining a number of physical properties that *do* depend on the chemical identity of the substance. In this chapter, the nature of these interactions and their effects on various physical properties of liquid and solid phases will be examined.

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3.1.2: Intermolecular Forces

Learning Objectives

- Describe the types of intermolecular forces possible between atoms or molecules in condensed phases (dispersion forces, dipole-dipole attractions, and hydrogen bonding)
- Identify the types of intermolecular forces experienced by specific molecules based on their structures
- Explain the relation between the intermolecular forces present within a substance and the temperatures associated with changes in its physical state

As was the case for gaseous substances, the kinetic molecular theory may be used to explain the behavior of solids and liquids. In the following description, the term *particle* will be used to refer to an atom, molecule, or ion. Note that we will use the popular phrase “intermolecular attraction” to refer to attractive forces between the particles of a substance, regardless of whether these particles are molecules, atoms, or ions.

Consider these two aspects of the molecular-level environments in solid, liquid, and gaseous matter:

- Particles in a solid are tightly packed together and often arranged in a regular pattern; in a liquid, they are close together with no regular arrangement; in a gas, they are far apart with no regular arrangement.
- Particles in a solid vibrate about fixed positions and do not generally move in relation to one another; in a liquid, they move past each other but remain in essentially constant contact; in a gas, they move independently of one another except when they collide.

The differences in the properties of a solid, liquid, or gas reflect the strengths of the attractive forces between the atoms, molecules, or ions that make up each phase. The phase in which a substance exists depends on the relative extents of its intermolecular forces (IMFs) and the kinetic energies (KE) of its molecules. IMFs are the various forces of attraction that may exist between the atoms and molecules of a substance due to electrostatic phenomena, as will be detailed in this module. These forces serve to hold particles close together, whereas the particles’ KE provides the energy required to overcome the attractive forces and thus increase the distance between particles. Figure 3.1.2.1 illustrates how changes in physical state may be induced by changing the temperature, hence, the average KE, of a given substance.

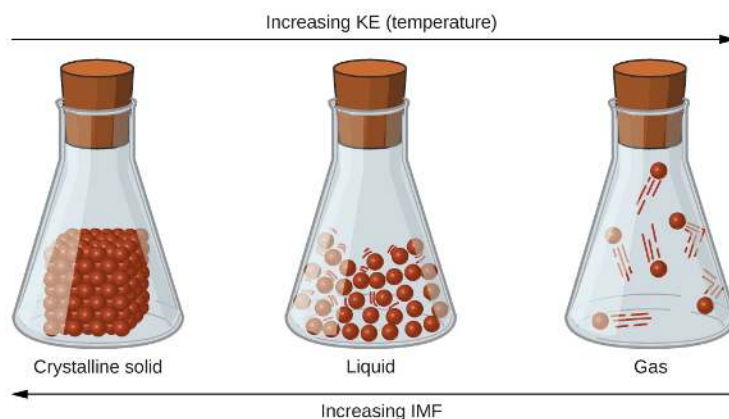
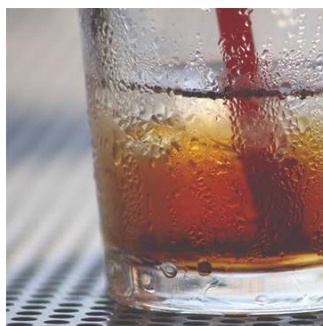


Figure 3.1.2.1: Transitions between solid, liquid, and gaseous states of a substance occur when conditions of temperature or pressure favor the associated changes in intermolecular forces. (Note: The space between particles in the gas phase is much greater than shown.)

Three sealed flasks are labeled, “Crystalline solid,” “Liquid,” and “Gas,” from left to right. The first flask holds a cube composed of small spheres sitting on the bottom while the second flask shows a lot of small spheres in the bottom that are spaced a small distance apart from one another and have lines around them to indicate motion. The third flask shows a few spheres spread far from one another with larger lines to indicate motion. There is a right-facing arrow that spans the top of all three flasks. The arrow is labeled, “Increasing K E (temperature).” There is a left-facing arrow that spans the bottom of all three flasks. The arrow is labeled, “Increasing I M F.”

As an example of the processes depicted in this figure, consider a sample of water. When gaseous water is cooled sufficiently, the attractions between H_2O molecules will be capable of holding them together when they come into contact with each other; the gas condenses, forming liquid H_2O . For example, liquid water forms on the outside of a cold glass as the water vapor in the air is cooled by the cold glass, as seen in Figure 3.1.2.2



(a)



(b)

Figure 3.1.2.2: Condensation forms when water vapor in the air is cooled enough to form liquid water, such as (a) on the outside of a cold beverage glass or (b) in the form of fog. (credit a: modification of work by Jenny Downing; credit b: modification of work by Cory Zanker)

Image a shows a brown colored beverage in a glass with condensation on the outside. Image b shows a body of water with fog hovering above the surface of the water.

We can also liquefy many gases by compressing them, if the temperature is not too high. The increased pressure brings the molecules of a gas closer together, such that the attractions between the molecules become strong relative to their KE. Consequently, they form liquids. Butane, C_4H_{10} , is the fuel used in disposable lighters and is a gas at standard temperature and pressure. Inside the lighter's fuel compartment, the butane is compressed to a pressure that results in its condensation to the liquid state, as shown in Figure 3.1.2.3



Figure 3.1.2.3: Gaseous butane is compressed within the storage compartment of a disposable lighter, resulting in its condensation to the liquid state. (credit: modification of work by "Sam-Cat"/Flickr)

Finally, if the temperature of a liquid becomes sufficiently low, or the pressure on the liquid becomes sufficiently high, the molecules of the liquid no longer have enough KE to overcome the IMF between them, and a solid forms. A more thorough discussion of these and other changes of state, or phase transitions, is provided in a later module of this chapter.

Forces between Molecules

Under appropriate conditions, the attractions between all gas molecules will cause them to form liquids or solids. This is due to intermolecular forces, not *intramolecular* forces. *Intramolecular* forces are those *within* the molecule that keep the molecule together, for example, the bonds between the atoms. *Intermolecular* forces are the attractions *between* molecules, which determine many of the physical properties of a substance. Figure 3.1.2.4 illustrates these different molecular forces. The strengths of these attractive forces vary widely, though usually the IMFs between small molecules are weak compared to the intramolecular forces

that bond atoms together within a molecule. For example, to overcome the IMFs in one mole of liquid HCl and convert it into gaseous HCl requires only about 17 kilojoules. However, to break the covalent bonds between the hydrogen and chlorine atoms in one mole of HCl requires about 25 times more energy—430 kilojoules.

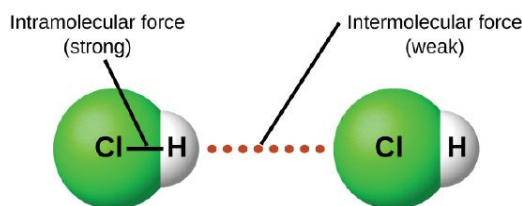


Figure 3.1.2.4: Intramolecular forces keep a molecule intact. Intermolecular forces hold multiple molecules together and determine many of a substance's properties.

An image is shown in which two molecules composed of a green sphere labeled “C l” connected on the right to a white sphere labeled “H” are near one another with a dotted line labeled “Intermolecular force (weak)” drawn between them. A line connects the two spheres in each molecule and the line is labeled “Intramolecular force (strong).”

All of the attractive forces between neutral atoms and molecules are known as van der Waals forces, although they are usually referred to more informally as intermolecular attraction. We will consider the various types of IMFs in the next three sections of this module.

Dispersion Forces

One of the three van der Waals forces is present in all condensed phases, regardless of the nature of the atoms or molecules composing the substance. This attractive force is called the London dispersion force in honor of German-born American physicist Fritz London who, in 1928, first explained it. This force is often referred to as simply the dispersion force. Because the electrons of an atom or molecule are in constant motion (or, alternatively, the electron's location is subject to quantum-mechanical variability), at any moment in time, an atom or molecule can develop a temporary, instantaneous dipole if its electrons are distributed asymmetrically. The presence of this dipole can, in turn, distort the electrons of a neighboring atom or molecule, producing an induced dipole. These two rapidly fluctuating, temporary dipoles thus result in a relatively weak electrostatic attraction between the species—a so-called dispersion force like that illustrated in Figure 3.1.2.5

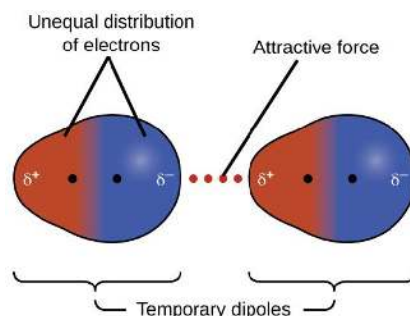


Figure 3.1.2.5: Dispersion forces result from the formation of temporary dipoles, as illustrated here for two nonpolar diatomic molecules.

Two pairs of molecules are shown where each molecule has one larger blue side labeled “delta sign, negative sign” and a smaller red side labeled “delta sign, positive sign.” Toward the middle of the both molecules, but still on each distinct side, is a black dot. Between the two images is a dotted line labeled, “Attractive force.” In the first image, the red and blue sides are labeled, “Unequal distribution of electrons.” Below both images are brackets. The brackets are labeled, “Temporary dipoles.”

Dispersion forces that develop between atoms in different molecules can attract the two molecules to each other. The forces are relatively weak, however, and become significant only when the molecules are very close. Larger and heavier atoms and molecules exhibit stronger dispersion forces than do smaller and lighter atoms and molecules. F_2 and Cl_2 are gases at room temperature (reflecting weaker attractive forces); Br_2 is a liquid, and I_2 is a solid (reflecting stronger attractive forces). Trends in observed melting and boiling points for the halogens clearly demonstrate this effect, as seen in Table 3.1.2.1.

Table 3.1.2.1: Melting and Boiling Points of the Halogens

Halogen	Molar Mass	Atomic Radius	Melting Point	Boiling Point
fluorine, F_2	38 g/mol	72 pm	53 K	85 K

Halogen	Molar Mass	Atomic Radius	Melting Point	Boiling Point
chlorine, Cl ₂	71 g/mol	99 pm	172 K	238 K
bromine, Br ₂	160 g/mol	114 pm	266 K	332 K
iodine, I ₂	254 g/mol	133 pm	387 K	457 K
astatine, At ₂	420 g/mol	150 pm	575 K	610 K

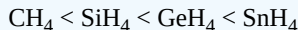
The increase in melting and boiling points with increasing atomic/molecular size may be rationalized by considering how the strength of dispersion forces is affected by the electronic structure of the atoms or molecules in the substance. In a larger atom, the valence electrons are, on average, farther from the nuclei than in a smaller atom. Thus, they are less tightly held and can more easily form the temporary dipoles that produce the attraction. The measure of how easy or difficult it is for another electrostatic charge (for example, a nearby ion or polar molecule) to distort a molecule's charge distribution (its electron cloud) is known as polarizability. A molecule that has a charge cloud that is easily distorted is said to be very polarizable and will have large dispersion forces; one with a charge cloud that is difficult to distort is not very polarizable and will have small dispersion forces.

✓ Example 3.1.2.1: London Forces and Their Effects

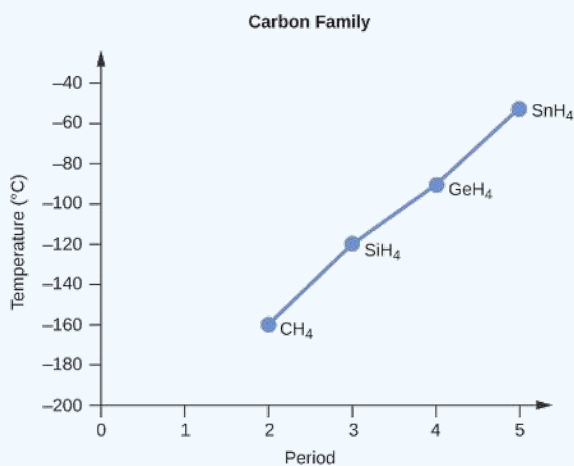
Order the following compounds of a group 14 element and hydrogen from lowest to highest boiling point: CH₄, SiH₄, GeH₄, and SnH₄. Explain your reasoning.

Solution

Applying the skills acquired in the chapter on chemical bonding and molecular geometry, all of these compounds are predicted to be nonpolar, so they may experience only dispersion forces: the smaller the molecule, the less polarizable and the weaker the dispersion forces; the larger the molecule, the larger the dispersion forces. The molar masses of CH₄, SiH₄, GeH₄, and SnH₄ are approximately 16 g/mol, 32 g/mol, 77 g/mol, and 123 g/mol, respectively. Therefore, CH₄ is expected to have the lowest boiling point and SnH₄ the highest boiling point. The ordering from lowest to highest boiling point is expected to be



A graph of the actual boiling points of these compounds versus the period of the group 14 elements shows this prediction to be correct:



A line graph, titled "Carbon Family," is shown where the y-axis is labeled "Temperature, (degree sign C)" and has values of "negative 200" to "negative 40" from bottom to top in increments of 20. The x-axis is labeled "Period" and has values of "0" to "5" in increments of 1. The first point on the graph is labeled "C H subscript 4" and is at point "2, negative 160." The second point on the graph is labeled "S i H subscript 4" and is at point "3, negative 120" while the third point on the graph is labeled "G e H subscript 4" and is at point "4, negative 100." The fourth point on the graph is labeled "S n H subscript 4" and is at point "5, negative 60."

? Exercise 3.1.2.1

Order the following hydrocarbons from lowest to highest boiling point: C_2H_6 , C_3H_8 , and C_4H_{10} .

Answer

All of these compounds are nonpolar and only have London dispersion forces: the larger the molecule, the larger the dispersion forces and the higher the boiling point. The ordering from lowest to highest boiling point is therefore



The shapes of molecules also affect the magnitudes of the dispersion forces between them. For example, boiling points for the isomers *n*-pentane, isopentane, and neopentane (shown in Figure 3.1.2.6) are 36 °C, 27 °C, and 9.5 °C, respectively. Even though these compounds are composed of molecules with the same chemical formula, C_5H_{12} , the difference in boiling points suggests that dispersion forces in the liquid phase are different, being greatest for *n*-pentane and least for neopentane. The elongated shape of *n*-pentane provides a greater surface area available for contact between molecules, resulting in correspondingly stronger dispersion forces. The more compact shape of isopentane offers a smaller surface area available for intermolecular contact and, therefore, weaker dispersion forces. Neopentane molecules are the most compact of the three, offering the least available surface area for intermolecular contact and, hence, the weakest dispersion forces. This behavior is analogous to the connections that may be formed between strips of VELCRO brand fasteners: the greater the area of the strip's contact, the stronger the connection.

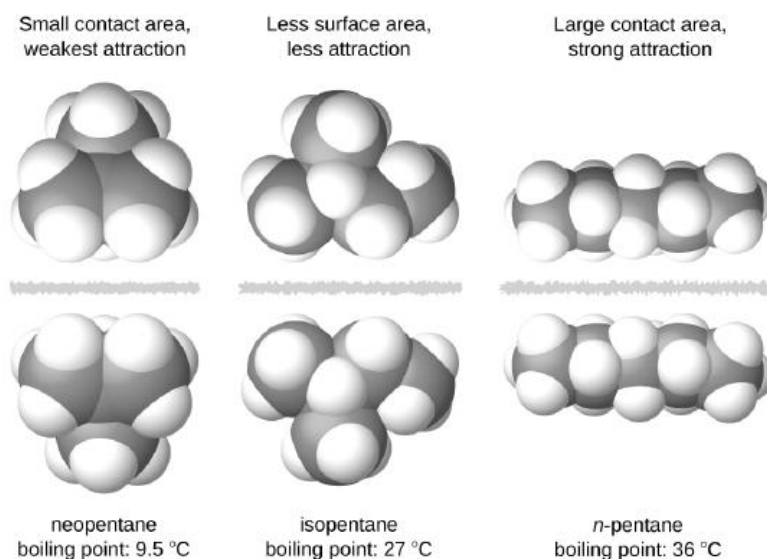


Figure 3.1.2.6: The strength of the dispersion forces increases with the contact area between molecules, as demonstrated by the boiling points of these pentane isomers.

Three images of molecules are shown. The first shows a cluster of large, gray spheres each bonded together and to several smaller, white spheres. There is a gray, jagged line and then the mirror image of the first cluster of spheres is shown. Above these two clusters is the label, "Small contact area, weakest attraction," and below is the label, "neopentane boiling point: 9.5 degrees C." The second shows a chain of three gray spheres bonded by the middle sphere to a fourth gray sphere. Each gray sphere is bonded to several smaller, white spheres. There is a jagged, gray line and then the mirror image of the first chain appears. Above these two chains is the label, "Less surface area, less attraction," and below is the label, "isopentane boiling point: 27 degrees C." The third image shows a chain of five gray spheres bonded together and to several smaller, white spheres. There is a jagged gray line and then the mirror image of the first chain appears. Above these chains is the label, "Large contact area, strong attraction," and below is the label, "n-pentane boiling point 36 degrees C."

📌 Applications: Geckos and Intermolecular Forces

Geckos have an amazing ability to adhere to most surfaces. They can quickly run up smooth walls and across ceilings that have no toe-holds, and they do this without having suction cups or a sticky substance on their toes. And while a gecko can lift its feet easily as it walks along a surface, if you attempt to pick it up, it sticks to the surface. How are geckos (as well as spiders and some other insects) able to do this? Although this phenomenon has been investigated for hundreds of years, scientists only recently uncovered the details of the process that allows geckos' feet to behave this way.

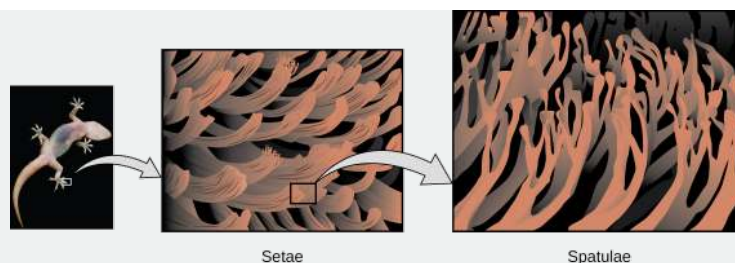
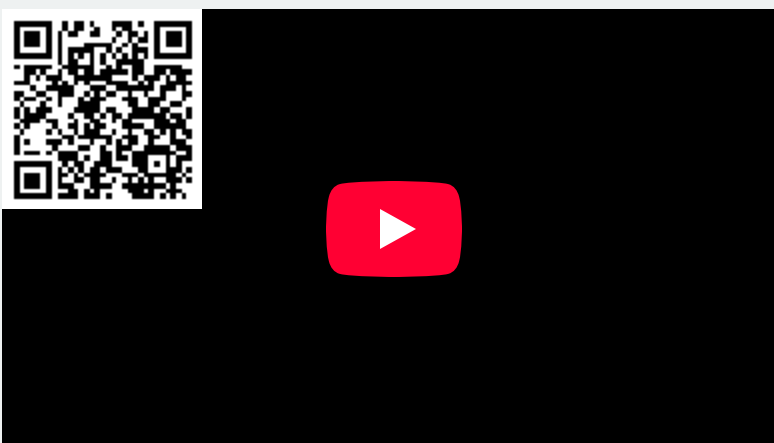


Figure 3.1.2.7: Geckos' toes contain large numbers of tiny hairs (setae), which branch into many triangular tips (spatulae). Geckos adhere to surfaces because of van der Waals attractions between the surface and a gecko's millions of spatulae. By changing how the spatulae contact the surface, geckos can turn their stickiness "on" and "off." (credit photo: modification of work by "JC*+A!" / Flickr)

Three figures are shown. The first is a photo of the bottom of a gecko's foot. The second is bigger version which shows the setae. The third is a bigger version of the setae and shows the spatulae.

Geckos' toes are covered with hundreds of thousands of tiny hairs known as *setae*, with each seta, in turn, branching into hundreds of tiny, flat, triangular tips called *spatulae*. The huge numbers of spatulae on its setae provide a gecko, shown in Figure 3.1.2.7, with a large total surface area for sticking to a surface. In 2000, Kellar Autumn, who leads a multi-institutional gecko research team, found that geckos adhered equally well to both polar silicon dioxide and nonpolar gallium arsenide. This proved that geckos stick to surfaces because of dispersion forces—weak intermolecular attractions arising from temporary, synchronized charge distributions between adjacent molecules. Although dispersion forces are very weak, the total attraction over millions of spatulae is large enough to support many times the gecko's weight.

In 2014, two scientists developed a model to explain how geckos can rapidly transition from "sticky" to "non-sticky." Alex Greaney and Congcong Hu at Oregon State University described how geckos can achieve this by changing the angle between their spatulae and the surface. Geckos' feet, which are normally nonsticky, become sticky when a small shear force is applied. By curling and uncurling their toes, geckos can alternate between sticking and unsticking from a surface, and thus easily move across it. Further investigations may eventually lead to the development of better adhesives and other applications.



Watch this video to learn more about Kellar Autumn's research that determined that van der Waals forces are responsible for a gecko's ability to cling and climb.

Dipole-Dipole Attractions

Recall from the chapter on chemical bonding and molecular geometry that *polar* molecules have a partial positive charge on one side and a partial negative charge on the other side of the molecule—a separation of charge called a *dipole*. Consider a polar molecule such as hydrogen chloride, HCl. In the HCl molecule, the more electronegative Cl atom bears the partial negative charge, whereas the less electronegative H atom bears the partial positive charge. An attractive force between HCl molecules results from the attraction between the positive end of one HCl molecule and the negative end of another. This attractive force is called a dipole-dipole attraction—the electrostatic force between the partially positive end of one polar molecule and the partially negative end of another, as illustrated in Figure 3.1.2.8

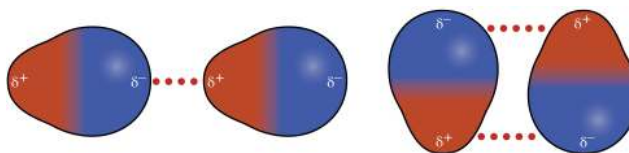


Figure 3.1.2.8: This image shows two arrangements of polar molecules, such as HCl, that allow an attraction between the partial negative end of one molecule and the partial positive end of another.

Two pairs of molecules are shown where each molecule has one larger blue side labeled “delta sign, negative sign” and a smaller red side labeled “delta sign, positive sign. In the first pair, the red sides of the two molecules both face to the left and the blue side to the right. A horizontal dotted line lies in between the two. In the second pair, the molecules face up and down, with the red and blue ends aligning. A horizontal dotted line lies between the red and blue ends facing upward and another lies between the red and blue ends facing downward.

The effect of a dipole-dipole attraction is apparent when we compare the properties of HCl molecules to nonpolar F_2 molecules. Both HCl and F_2 consist of the same number of atoms and have approximately the same molecular mass. At a temperature of 150 K, molecules of both substances would have the same average KE. However, the dipole-dipole attractions between HCl molecules are sufficient to cause them to “stick together” to form a liquid, whereas the relatively weaker dispersion forces between nonpolar F_2 molecules are not, and so this substance is gaseous at this temperature. The higher normal boiling point of HCl (188 K) compared to F_2 (85 K) is a reflection of the greater strength of dipole-dipole attractions between HCl molecules, compared to the attractions between nonpolar F_2 molecules. We will often use values such as boiling or freezing points, or enthalpies of vaporization or fusion, as indicators of the relative strengths of IMFs of attraction present within different substances.

✓ Example 3.1.2.2: Dipole-Dipole Forces and Their Effects

Predict which will have the higher boiling point: N_2 or CO. Explain your reasoning.

Solution

CO and N_2 are both diatomic molecules with masses of about 28 amu, so they experience similar London dispersion forces. Because CO is a polar molecule, it experiences dipole-dipole attractions. Because N_2 is nonpolar, its molecules cannot exhibit dipole-dipole attractions. The dipole-dipole attractions between CO molecules are comparably stronger than the dispersion forces between nonpolar N_2 molecules, so CO is expected to have the higher boiling point.

A common method for preparing oxygen is the decomposition

? Exercise 3.1.2.2

Predict which will have the higher boiling point: ICl or Br_2 . Explain your reasoning.

Answer

ICl. ICl and Br_2 have similar masses (~160 amu) and therefore experience similar London dispersion forces. ICl is polar and thus also exhibits dipole-dipole attractions; Br_2 is nonpolar and does not. The relatively stronger dipole-dipole attractions require more energy to overcome, so ICl will have the higher boiling point.

Hydrogen Bonding

Nitrosyl fluoride (ONF, molecular mass 49 amu) is a gas at room temperature. Water (H_2O , molecular mass 18 amu) is a liquid, even though it has a lower molecular mass. We clearly cannot attribute this difference between the two compounds to dispersion forces. Both molecules have about the same shape and ONF is the heavier and larger molecule. It is, therefore, expected to experience more significant dispersion forces. Additionally, we cannot attribute this difference in boiling points to differences in the dipole moments of the molecules. Both molecules are polar and exhibit comparable dipole moments. The large difference between the boiling points is due to a particularly strong dipole-dipole attraction that may occur when a molecule contains a hydrogen atom bonded to a fluorine, oxygen, or nitrogen atom (the three most electronegative elements). The very large difference in electronegativity between the H atom (2.1) and the atom to which it is bonded (4.0 for an F atom, 3.5 for an O atom, or 3.0 for a N atom), combined with the very small size of a H atom and the relatively small sizes of F, O, or N atoms, leads to *highly concentrated partial charges* with these atoms. Molecules with F-H, O-H, or N-H moieties are very strongly attracted to similar

moieties in nearby molecules, a particularly strong type of dipole-dipole attraction called hydrogen bonding. Examples of hydrogen bonds include $\text{HF} \cdots \text{HF}$, $\text{H}_2\text{O} \cdots \text{HOH}$, and $\text{H}_3\text{N} \cdots \text{HNH}_2$, in which the hydrogen bonds are denoted by dots. Figure 3.1.2.9 illustrates hydrogen bonding between water molecules.

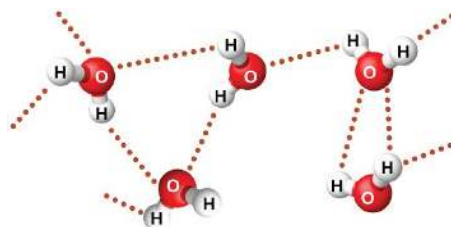


Figure 3.1.2.9: Water molecules participate in multiple hydrogen-bonding interactions with nearby water molecules.

Five water molecules are shown near one another, but not touching. A dotted line lies between many of the hydrogen atoms on one molecule and the oxygen atom on another molecule.

Despite use of the word “bond,” keep in mind that hydrogen bonds are *intermolecular* attractive forces, not *intramolecular* attractive forces (covalent bonds). Hydrogen bonds are much weaker than covalent bonds, only about 5 to 10% as strong, but are generally much stronger than other dipole-dipole attractions and dispersion forces.

Hydrogen bonds have a pronounced effect on the properties of condensed phases (liquids and solids). For example, consider the trends in boiling points for the binary hydrides of group 15 (NH_3 , PH_3 , AsH_3 , and SbH_3), group 16 hydrides (H_2O , H_2S , H_2Se , and H_2Te), and group 17 hydrides (HF , HCl , HBr , and HI). The boiling points of the heaviest three hydrides for each group are plotted in Figure 3.1.2.10. As we progress down any of these groups, the polarities of the molecules decrease slightly, whereas the sizes of the molecules increase substantially. The effect of increasingly stronger dispersion forces dominates that of increasingly weaker dipole-dipole attractions, and the boiling points are observed to increase steadily. For the group 15, 16, and 17 hydrides, the boiling points for each class of compounds increase with increasing molecular mass for elements in periods 3, 4, and 5.

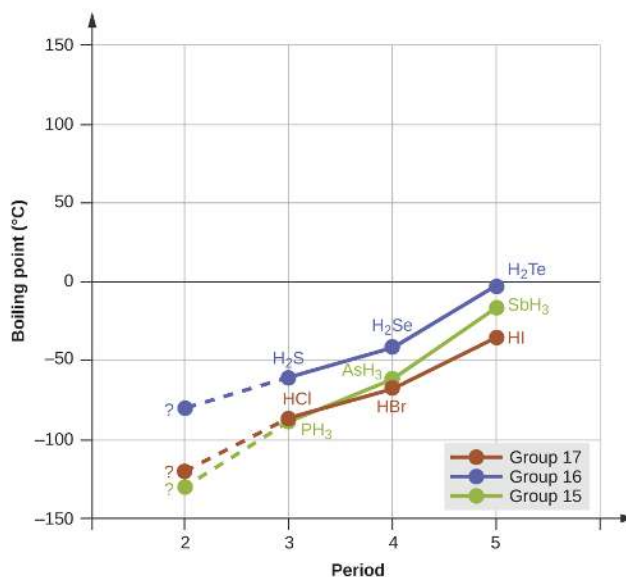


Figure 3.1.2.10: In comparison to periods 3–5, the binary hydrides of period 2 elements in groups 17, 16 and 15 (F, O and N, respectively) exhibit anomalously high boiling points due to hydrogen bonding.

A line graph is shown where the y-axis is labeled “Boiling point (, degree sign, C)” and has values of “negative 150” to “150” from bottom to top in increments of 50. The x-axis is labeled “Period” and has values of “0” to “5” in increments of 1. Three lines are shown on the graph and are labeled in the legend. The red line is labeled as “halogen family,” the blue is “oxygen family” and the green is “nitrogen family.” The first point on the red line is labeled “question mark” and is at point “2, negative 120.” The second point on the line is labeled “H C I” and is at point “3, negative 80” while the third point on the line is labeled “H B r” and is at point “4, negative 60.” The fourth point on the line is labeled “H I” and is at point “5, negative 40.” The first point on the green line is labeled “question mark” and is at point “2, negative 125.” The second point on the line is labeled “P H, subscript 3” and is at point “3, negative 80” while the third point on the line is labeled “A s H, subscript 3” and is at point “4, negative 55.” The fourth point on the line is labeled “S b H, subscript 3” and is at point “5, negative 10.” The first point on the blue line is labeled “question mark” and is at point “2, negative 80.” The second point on the line is labeled “H, subscript 2, S” and is at point “3, negative 55” while the third point on the line is labeled “H, subscript 2, S e” and is at point “4, negative 45.” The fourth point on the line is labeled “H, subscript 2, T e” and is at point “5, negative 3.”

If we use this trend to predict the boiling points for the lightest hydride for each group, we would expect NH_3 to boil at about -120°C , H_2O to boil at about -80°C , and HF to boil at about -110°C . However, when we measure the boiling points for these compounds, we find that they are dramatically higher than the trends would predict, as shown in Figure 3.1.2.10. The stark contrast between our naïve predictions and reality provides compelling evidence for the strength of hydrogen bonding.

✓ Example 3.1.2.3: Effect of Hydrogen Bonding on Boiling Points

Consider the compounds dimethylether (CH_3OCH_3), ethanol ($\text{CH}_3\text{CH}_2\text{OH}$), and propane ($\text{CH}_3\text{CH}_2\text{CH}_3$). Their boiling points, not necessarily in order, are -42.1°C , -24.8°C , and 78.4°C . Match each compound with its boiling point. Explain your reasoning.

Solution

The VSEPR-predicted shapes of CH_3OCH_3 , $\text{CH}_3\text{CH}_2\text{OH}$, and $\text{CH}_3\text{CH}_2\text{CH}_3$ are similar, as are their molar masses (46 g/mol, 46 g/mol, and 44 g/mol, respectively), so they will exhibit similar dispersion forces. Since $\text{CH}_3\text{CH}_2\text{CH}_3$ is nonpolar, it may exhibit *only* dispersion forces. Because CH_3OCH_3 is polar, it will also experience dipole-dipole attractions. Finally, $\text{CH}_3\text{CH}_2\text{OH}$ has an $-\text{OH}$ group, and so it will experience the uniquely strong dipole-dipole attraction known as hydrogen bonding. So the ordering in terms of strength of IMFs, and thus boiling points, is $\text{CH}_3\text{CH}_2\text{CH}_3 < \text{CH}_3\text{OCH}_3 < \text{CH}_3\text{CH}_2\text{OH}$. The boiling point of propane is -42.1°C , the boiling point of dimethylether is -24.8°C , and the boiling point of ethanol is 78.5°C .

? Exercise 3.1.2.3

Ethane (CH_3CH_3) has a melting point of -183°C and a boiling point of -89°C . Predict the melting and boiling points for methylamine (CH_3NH_2). Explain your reasoning.

Answer

The melting point and boiling point for methylamine are predicted to be significantly greater than those of ethane. CH_3CH_3 and CH_3NH_2 are similar in size and mass, but methylamine possesses an $-\text{NH}$ group and therefore may exhibit hydrogen bonding. This greatly increases its IMFs, and therefore its melting and boiling points. It is difficult to predict values, but the known values are a melting point of -93°C and a boiling point of -6°C .

Hydrogen Bonding and DNA

Deoxyribonucleic acid (DNA) is found in every living organism and contains the genetic information that determines the organism's characteristics, provides the blueprint for making the proteins necessary for life, and serves as a template to pass this information on to the organism's offspring. A DNA molecule consists of two (anti-)parallel chains of repeating nucleotides, which form its well-known double helical structure, as shown in Figure 3.1.2.10.

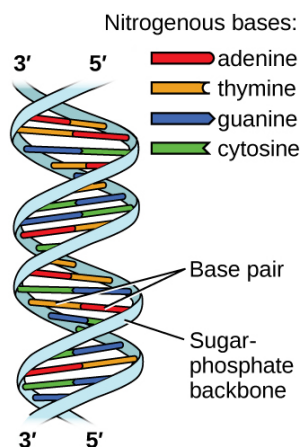


Figure 3.1.2.11: Two separate DNA molecules form a double-stranded helix in which the molecules are held together via hydrogen bonding. (credit: modification of work by Jerome Walker, Dennis Myts)

Two images are shown. The first lies on the left side of the page and shows a helical structure like a twisted ladder where the rungs of the ladder, labeled “Base pair” are red, yellow, green and blue paired bars. The red and yellow bars, which are always paired together, are labeled in the legend, which is titled “Nitrogenous bases” as “adenine” and “thymine,” respectively. The blue and green bars, which are always paired together, are labeled in the legend as “guanine” and “cytosine,” respectively. At the top of the helical structure, the left-hand side rail, or “Sugar, dash, phosphate backbone,” is labeled as “3, prime” while the right is labeled as “5, prime.” These labels are reversed at the bottom of the helix. To the right of the page is a large Lewis structure. The top left corner of this structure, labeled “5, prime,” shows a phosphorus atom single bonded to three oxygen atoms, one of which has a superscripted negative charge, and double bonded to a fourth oxygen atom. One of the single bonded oxygen atoms is single bonded to the left corner of a five-membered ring with an oxygen atom at its top point and which is single bonded to an oxygen atom on the bottom left. This oxygen atom is single bonded to a phosphorus atom that is single bonded to two other hydrogen atoms and double bonded to a fourth oxygen atom. The lower left of these oxygen atoms is single bonded to another oxygen atom that is single bonded to a five-membered ring with an oxygen in the upper bonding site. The bottom left of this ring has a hydroxyl group attached to it while the upper right carbon is single bonded to a nitrogen atom that is part of a five-membered ring bonded to a six-membered ring. Both of these rings have points of unsaturation and nitrogen atoms bonded into their structures. On the right side of the six-membered ring are two single bonded amine groups and a double bonded oxygen. Three separate dotted lines extend from these sites to corresponding sites on a second six-membered ring. This ring has points of unsaturation and a nitrogen atom in the bottom right bonding position that is single bonded to a five-membered ring on the right side of the image. This ring is single bonded to a carbon that is single bonded to an oxygen that is single bonded to a phosphorus. The phosphorus is single bonded to two other oxygen atoms and double bonded to a fourth oxygen atom. This group is labeled “5, prime.” The five-membered ring is also bonded on the top side to an oxygen that is bonded to a phosphorus single bonded to two other oxygen atoms and double bonded to a fourth oxygen atom. The upper left oxygen of this group is single bonded to a carbon that is single bonded to a five-membered ring with an oxygen in the bottom bonding position. This ring has a hydroxyl group on its upper right side that is labeled “3, prime” and is bonded on the left side to a nitrogen that is a member of a five-membered ring. This ring is bonded to a six-membered ring and both have points of unsaturation. This ring has a nitrogen on the left side, as well as an amine group, that have two dotted lines leading from them to an oxygen and amine group on a six membered ring. These dotted lines are labeled “Hydrogen bonds.” The six membered ring also has a double bonded oxygen on its lower side and a nitrogen atom on its left side that is single bonded to a five-membered ring. This ring connects to the two phosphate groups mentioned at the start of this to form a large circle. The name “guanine” is written below the lower left side of this image while the name “cytosine” is written on the lower right. The name “thymine” is written above the right side of the image and “adenine” is written on the top right. Three sections are indicated below the images where the left is labeled “Sugar, dash, phosphate backbone,” the middle is labeled “Bases” and the right is labeled “Sugar, dash, phosphate backbone.”

Each nucleotide contains a (deoxyribose) sugar bound to a phosphate group on one side, and one of four nitrogenous bases on the other. Two of the bases, cytosine (C) and thymine (T), are single-ringed structures known as pyrimidines. The other two, adenine (A) and guanine (G), are double-ringed structures called purines. These bases form complementary base pairs consisting of one purine and one pyrimidine, with adenine pairing with thymine, and cytosine with guanine. Each base pair is held together by hydrogen bonding. A and T share two hydrogen bonds, C and G share three, and both pairings have a similar shape and structure

Figure 3.1.2.12

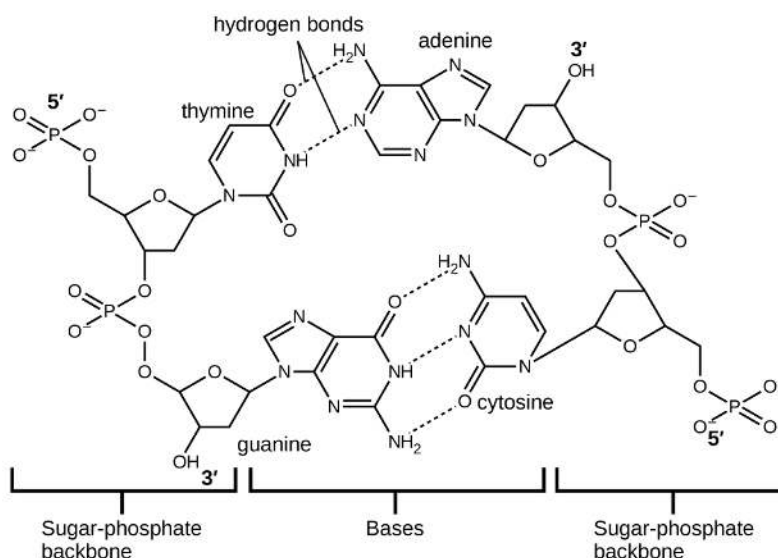


Figure 3.1.2.12: The geometries of the base molecules result in maximum hydrogen bonding between adenine and thymine (AT) and between guanine and cytosine (GC), so-called “complementary base pairs.”

A large Lewis structure is shown. The top left corner of this structure, labeled “5, prime,” shows a phosphorus atom single bonded to three oxygen atoms, one of which has a superscripted negative charge, and double bonded to a fourth oxygen atom. One of the single bonded oxygen atoms is single bonded to the left corner of a five-membered ring with an oxygen atom at its top point and which is single bonded to an oxygen atom on the bottom left. This oxygen atom is single bonded to a phosphorus atom that is single bonded to two other hydrogen atoms and double bonded to a fourth oxygen atom. The lower left of these oxygen atoms is single bonded to another oxygen atom that is single bonded to a five-membered ring with an oxygen in the upper bonding site. The bottom left of this ring has a hydroxyl group attached to it while the upper right carbon is single bonded to a nitrogen atom that is part of a five-membered ring bonded to a six-membered ring. Both of these rings have points of unsaturation and nitrogen atoms bonded into their structures. On the right side of the six-membered ring are two single bonded amine groups and a double bonded oxygen. Three separate dotted lines extend from these sites to corresponding sites on a second six-membered ring. This ring has points of unsaturation and a nitrogen atom in the bottom right bonding position that is single bonded to a five-membered ring on the right side of the image. This ring is single bonded to a carbon that is single bonded to an oxygen that is single bonded to a phosphorus. The phosphorus is single bonded to two other oxygen atoms and double bonded to a fourth oxygen atom. This group is labeled “5, prime.” The five-membered ring is also bonded on the top side to an oxygen that is bonded to a phosphorus single bonded to two other oxygen atoms and double bonded to a fourth oxygen atom. The upper left oxygen of this group is single bonded to a carbon that is single bonded to a five-membered ring with an oxygen in the bottom bonding position. This ring has a hydroxyl group on its upper right side that is labeled “3, prime” and is bonded on the left side to a nitrogen that is a member of a five-membered ring. This ring is bonded to a six-membered ring and both have points of unsaturation. This ring has a nitrogen on the left side, as well as an amine group, that have two dotted lines leading from them to an oxygen and amine group on a six membered ring. These dotted lines are labeled “Hydrogen bonds.” The six membered ring also has a double bonded oxygen on its lower side and a nitrogen atom on its left side that is single bonded to a five-membered ring. This ring connects to the two phosphate groups mentioned at the start of this to form a large circle. The name “guanine” is written below the lower left side of this image while the name “cytosine” is written on the lower right. The name “thymine” is written above the right side of the image and “adenine” is written on the top right. Three sections are indicated below the images where the left is labeled “Sugar, dash, phosphate backbone,” the middle is labeled “Bases” and the right is labeled “Sugar, dash, phosphate backbone.”

The cumulative effect of millions of hydrogen bonds effectively holds the two strands of DNA together. Importantly, the two strands of DNA can relatively easily “unzip” down the middle since hydrogen bonds are relatively weak compared to the covalent bonds that hold the atoms of the individual DNA molecules together. This allows both strands to function as a template for replication.

Summary

The physical properties of condensed matter (liquids and solids) can be explained in terms of the kinetic molecular theory. In a liquid, intermolecular attractive forces hold the molecules in contact, although they still have sufficient kinetic energy to move past each other. Intermolecular attractive forces, collectively referred to as van der Waals forces, are responsible for the behavior of liquids and solids and are electrostatic in nature. Dipole-dipole attractions result from the electrostatic attraction of the partial negative end of one dipolar molecule for the partial positive end of another. The temporary dipole that results from the motion of the electrons in an atom can induce a dipole in an adjacent atom and give rise to the London dispersion force. London forces increase with increasing molecular size. Hydrogen bonds are a special type of dipole-dipole attraction that results when hydrogen is bonded to one of the three most electronegative elements: F, O, or N.

Glossary

dipole-dipole attraction

intermolecular attraction between two permanent dipoles

dispersion force

(also, London dispersion force) attraction between two rapidly fluctuating, temporary dipoles; significant only when particles are very close together

hydrogen bonding

occurs when exceptionally strong dipoles attract; bonding that exists when hydrogen is bonded to one of the three most electronegative elements: F, O, or N

induced dipole

temporary dipole formed when the electrons of an atom or molecule are distorted by the instantaneous dipole of a neighboring atom or molecule

instantaneous dipole

temporary dipole that occurs for a brief moment in time when the electrons of an atom or molecule are distributed asymmetrically

intermolecular force

noncovalent attractive force between atoms, molecules, and/or ions

polarizability

measure of the ability of a charge to distort a molecule's charge distribution (electron cloud)

van der Waals force

attractive or repulsive force between molecules, including dipole-dipole, dipole-induced dipole, and London dispersion forces; does not include forces due to covalent or ionic bonding, or the attraction between ions and molecules

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3.1.3: Forces in Solutions

Learning Objectives

- Learn some terminology involving solutions.
- Explain the significance of the statement "like dissolves like".
- Explain why certain substances dissolve in other substances.

A **solution** is another name for a homogeneous mixture. A **mixture** as a material composed of two or more substances. In a solution, the combination is so intimate that the



Figure 3.1.3.1 Making a saline water solution by dissolving table salt (NaCl) in water. The salt is the solute and the water the solvent. (CC-BY-SA 3.0; Chris 73).

different substances cannot be differentiated by sight, even with a microscope. Compare, for example, a mixture of salt and pepper and another mixture consisting of salt and water. In the first mixture, we can readily see individual grains of salt and the flecks of pepper. A mixture of salt and pepper is not a solution. However, in the second mixture, no matter how carefully we look, we cannot see two different substances. Salt dissolved in water is a solution.

The major component of a solution, called the **solvent**, is typically the same phase as the solution itself. Each minor component of a solution (and there may be more than one) is called the **solute**. In most of the solutions we will describe in this textbook, there will be no ambiguity about whether a component is the solvent or the solute.) For example, in a solution of salt in water, the solute is salt, and solvent is water Figure 3.1.3.1.

Solutions come in all phases, and the solvent and the solute do not have to be in the same phase to form a solution (such as salt and water). For example, air is a gaseous solution of about 80% nitrogen and about 20% oxygen, with some other gases present in much smaller amounts. An alloy is a solid solution consisting of a metal (like iron) with some other metals or nonmetals dissolved in it. Steel, an alloy of iron and carbon and small amounts of other metals, is an example of a solid solution. Table 3.1.3.1 lists some common types of solutions, with examples of each.

Table 3.1.3.1 Types of Solutions

Solvent Phase	Solute Phase	Example
gas	gas	air
liquid	gas	carbonated beverages
liquid	liquid	ethanol (C ₂ H ₅ OH) in H ₂ O (alcoholic beverages)
liquid	solid	salt water
solid	gas	H ₂ gas absorbed by Pd metal
solid	liquid	Hg(l) in dental fillings
solid	solid	steel alloys

✓ Example 3.1.3.1: Sugar and Water

A solution is made by dissolving 1.00 g of sucrose ($C_{12}H_{22}O_{11}$) in 100.0 g of liquid water. Identify the solvent and solute in the resulting solution.

Solution

Either by mass or by moles, the obvious minor component is **sucrose**, so it is **the solute**. **Water**—the majority component—is **the solvent**. The fact that the resulting solution is the same phase as water also suggests that water is the solvent.

? Exercise 3.1.3.1

A solution is made by dissolving 3.33 g of $HCl(g)$ in 40.0 g of liquid methyl alcohol (CH_3OH). Identify the solvent and solute in the resulting solution.

Answer

solute: $HCl(g)$; solvent: CH_3OH

Like Dissolves Like

A simple way to predict which compounds will dissolve in other compounds is the phrase "like dissolves like". What this means is that polar compounds dissolve polar compounds, nonpolar compounds dissolve nonpolar compounds, but polar and nonpolar do not dissolve in each other.

Even some nonpolar substances dissolve in water but only to a limited degree. Have you ever wondered why fish are able to breathe? Oxygen gas, an nonpolar molecules, does dissolve in water and it is this oxygen that the fish take in through their gills. Or, one more example of a nonpolar compound that dissolves in water is the reason we can enjoy carbonated sodas. Pepsi-cola and all the other sodas have carbon dioxide gas, CO_2 , a nonpolar compound, dissolved in a sugar-water solution. In this case, to keep as much gas in solution as possible, the sodas are kept under pressure.

This general trend of "like dissolves like" is summarized in the following table:

Table 3.1.3.2 Summary of Solubilities

Solute	Solvent	Is Solution Formed?
Polar Covalent	Polar	yes
Non-polar Covalent	Non-polar	yes
Polar Covalent	Non-polar	no
Non-polar Covalent	Polar	no
Ionic	Polar	yes
Ionic	Non-polar	no

Note that every time charged particles (ionic compounds or polar substances) are mixed, a solution is formed. When particles with no charges (nonpolar compounds) are mixed, they will form a solution. However, if substances with charges are mixed with other substances without charges a solution does not form.

When an ionic compound is considered "insoluble", it doesn't necessarily mean the compound is completely untouched by water. All ionic compounds dissolve to some extent. An insoluble compound just doesn't dissolve in any noticeable or appreciable amount.

What is it that makes a solute soluble in some solvents but not others?

The answer is intermolecular interactions. The intermolecular interactions include London dispersion forces, dipole-dipole interactions, and hydrogen bonding (as described in



Figure 3.1.3.1 Making a saline water solution by dissolving table salt (NaCl) in water. The salt is the solute and the water the solvent. (CC-BY-SA 3.0; Chris 73).

the previous section). From experimental studies, it has been determined that if molecules of a solute experience the same intermolecular forces that the solvent does, the solute will likely dissolve in that solvent. So, NaCl—a very polar substance because it is composed of ions—dissolves in water, which is very polar, but not in oil, which is generally nonpolar. Nonpolar wax dissolves in nonpolar hexane, but not in polar water. *Liquids that dissolve in one another in all proportions are said to be **miscible**. Liquids that do not dissolve in one another are called **immiscible**.*

Figure 3.1.3.2 Water (clear liquid) and oil (yellow) do not form liquid solutions. (CC BY-SA 1.0 Generic; Victor Blacus)

✓ Example 3.1.3.2: Polar and Nonpolar Solvents

Would I₂ be more soluble in CCl₄ or H₂O? Explain your answer.

Solution

I₂ is nonpolar. Of the two solvents, CCl₄ is nonpolar and H₂O is polar, so I₂ would be expected to be more soluble in CCl₄.

? Exercise 3.1.3.2

Would C₃H₇OH be more soluble in CCl₄ or H₂O? Explain your answer.

Answer

H₂O because both experience hydrogen bonding

✓ Example 3.1.3.3

Water is considered a polar solvent. Which substances should dissolve in water?

- methanol (CH₃OH)
- sodium sulfate (Na₂SO₄)
- octane (C₈H₁₈)

Solution

Because water is polar, substances that are polar or ionic will dissolve in it.

- Because of the OH group in methanol, we expect its molecules to be polar. Thus, we expect it to be soluble in water. As both water and methanol are liquids, the word *miscible* can be used in place of *soluble*.
- Sodium sulfate is an ionic compound, so we expect it to be soluble in water.
- Like other hydrocarbons, octane is nonpolar, so we expect that it would not be soluble in water.

? Exercise 3.1.3.3

Toluene ($\text{C}_6\text{H}_5\text{CH}_3$) is widely used in industry as a nonpolar solvent. Which substances should dissolve in toluene?

- water (H_2O)
- sodium sulfate (Na_2SO_4)
- octane (C_8H_{18})

Answer

octane (C_8H_{18}) will dissolve. It is also non-polar.

The Dissolving Process

Water typically dissolves most ionic compounds and polar molecules. Nonpolar molecules, such as those found in grease or oil, do not dissolve in water. We will first examine the process that occurs when an ionic compound, such as table salt (sodium chloride), dissolves in water.

Water molecules move about continuously due to their kinetic energy. When a crystal of sodium chloride is placed into water, the water's molecules collide with the crystal lattice. Recall that the crystal lattice is composed of alternating positive and negative ions. Water is attracted to the sodium chloride crystal because water is polar; it has both a positive and a negative end. The positively charged sodium ions in the crystal attract the oxygen end of the water molecules because they are partially negative. The negatively charged chloride ions in the crystal attract the hydrogen end of the water molecules because they are partially positive. The action of the polar water molecules takes the crystal lattice apart (see figure below).

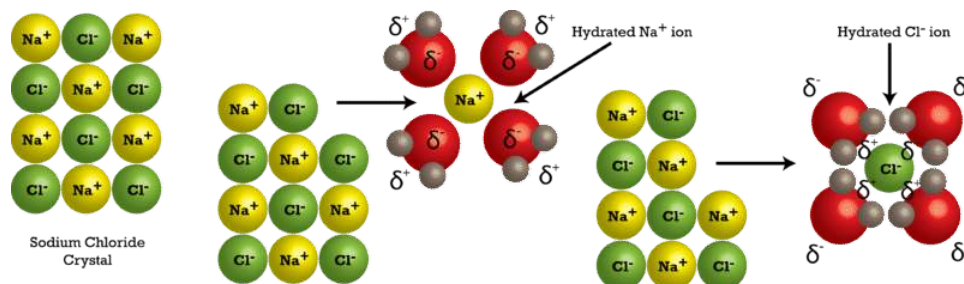


Figure 3.1.3.3: The process of an ionic sodium chloride crystal being dissolved and hydrated by water.

After coming apart from the crystal, the individual ions are then surrounded by solvent particles in a process called **solvation**. Note in the figure above that the individual Na^+ ions are surrounded by water molecules with the oxygen atom oriented near the positive ion. Likewise, the chloride ions are surrounded by water molecules with the opposite orientation. Thus, numerous **ion-dipole** interactions are formed. **Hydration** is the process of solute particles being surrounded by water molecules arranged in a specific manner. Hydration helps to stabilize aqueous solutions by preventing the positive and negative ions from coming back together and forming a precipitate.

Table sugar is made of the molecular compound sucrose ($\text{C}_{12}\text{H}_{22}\text{O}_{11}$). Solid sugar consists of individual sugar molecules held together by intermolecular attractive forces. When water dissolves sugar, it separates the individual sugar molecules by disrupting the attractive forces, but it *does not break the covalent bonds* between the carbon, hydrogen, and oxygen atoms. Dissolved sugar molecules are also hydrated. The hydration shell around a molecule of sucrose is arranged so that its partially negative oxygen atoms are near the partially positive hydrogen atoms in the solvent, and vice versa.

Summary

- Solutions are composed of a solvent (major component) and a solute (minor component).
- “Like dissolves like” is a useful rule for deciding if a solute will be soluble in a solvent.
- Liquids that dissolve in one another in all proportions are said to be **miscible**.
- Liquids that do not dissolve in one another are called **immiscible**.
- Ion-dipole** interactions are formed when ionic compounds dissolve in water.

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3.2: Separating Dissolved Components

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3.2.1: Solubility

Learning Objectives

- Describe the effects of temperature and pressure on solubility
- State Henry's law and use it in calculations involving the solubility of a gas in a liquid
- Explain the degrees of solubility possible for liquid-liquid solutions

Imagine adding a small amount of salt to a glass of water, stirring until all the salt has dissolved, and then adding a bit more. You can repeat this process until the salt concentration of the solution reaches its natural limit, a limit determined primarily by the relative strengths of the solute-solute, solute-solvent, and solvent-solvent attractive forces discussed in the previous two modules of this chapter. You can be certain that you have reached this limit because, no matter how long you stir the solution, undissolved salt remains. The concentration of salt in the solution at this point is known as its solubility.

The solubility of a solute in a particular solvent is the maximum concentration that may be achieved under given conditions when the dissolution process is at equilibrium. Referring to the example of salt in water:



When a solute's concentration is equal to its solubility, the solution is said to be saturated with that solute. If the solute's concentration is less than its solubility, the solution is said to be unsaturated. A solution that contains a relatively low concentration of solute is called dilute, and one with a relatively high concentration is called concentrated.

If we add more salt to a saturated solution of salt, we see it fall to the bottom and no more seems to dissolve. In fact, the added salt does dissolve, as represented by the forward direction of the dissolution equation. Accompanying this process, dissolved salt will precipitate, as depicted by the reverse direction of the equation. The system is said to be at equilibrium when these two reciprocal processes are occurring at equal rates, and so the amount of undissolved and dissolved salt remains constant. Support for the simultaneous occurrence of the dissolution and precipitation processes is provided by noting that the number and sizes of the undissolved salt crystals will change over time, though their combined mass will remain the same.



Video 3.2.1.1: Watch this impressive video showing the precipitation of sodium acetate from a supersaturated solution.

Solutions may be prepared in which a solute concentration exceeds its solubility. Such solutions are said to be supersaturated, and they are interesting examples of nonequilibrium states. For example, the carbonated beverage in an open container that has not yet “gone flat” is supersaturated with carbon dioxide gas; given time, the CO_2 concentration will decrease until it reaches its equilibrium value.

Solutions of Gases in Liquids

In an earlier module of this chapter, the effect of intermolecular attractive forces on solution formation was discussed. The chemical structures of the solute and solvent dictate the types of forces possible and, consequently, are important factors in determining solubility. For example, under similar conditions, the water solubility of oxygen is approximately three times greater than that of helium, but 100 times less than the solubility of chloromethane, CHCl_3 . Considering the role of the solvent's chemical

structure, note that the solubility of oxygen in the liquid hydrocarbon hexane, C_6H_{14} , is approximately 20 times greater than it is in water.

Other factors also affect the solubility of a given substance in a given solvent. Temperature is one such factor, with gas solubility typically decreasing as temperature increases (Figure 3.2.1.1). This is one of the major impacts resulting from the thermal pollution of natural bodies of water.

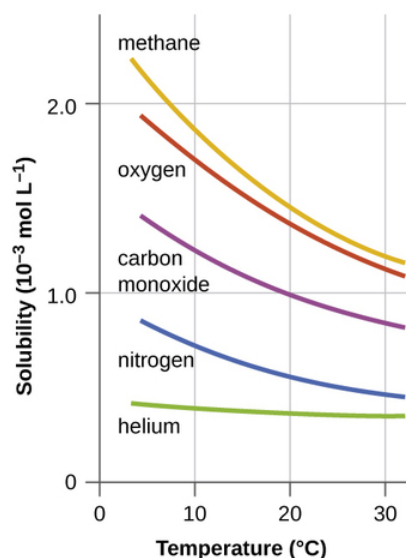


Figure 3.2.1.1: The solubilities of these gases in water decrease as the temperature increases. All solubilities were measured with a constant pressure of 101.3 kPa (1 atm) of gas above the solutions.

When the temperature of a river, lake, or stream is raised abnormally high, usually due to the discharge of hot water from some industrial process, the solubility of oxygen in the water is decreased. Decreased levels of dissolved oxygen may have serious consequences for the health of the water's ecosystems and, in severe cases, can result in large-scale fish kills (Figure 3.2.1.2).



Figure 3.2.1.2: (a) The small bubbles of air in this glass of chilled water formed when the water warmed to room temperature and the solubility of its dissolved air decreased. (b) The decreased solubility of oxygen in natural waters subjected to thermal pollution can result in large-scale fish kills. (credit a: modification of work by Liz West; credit b: modification of work by U.S. Fish and Wildlife Service)

The solubility of a gaseous solute is also affected by the partial pressure of solute in the gas to which the solution is exposed. Gas solubility increases as the pressure of the gas increases. Carbonated beverages provide a nice illustration of this relationship. The carbonation process involves exposing the beverage to a relatively high pressure of carbon dioxide gas and then sealing the beverage container, thus saturating the beverage with CO_2 at this pressure. When the beverage container is opened, a familiar hiss is heard as the carbon dioxide gas pressure is released, and some of the dissolved carbon dioxide is typically seen leaving solution in the form of small bubbles (Figure 3.2.1.3). At this point, the beverage is supersaturated with carbon dioxide and, with time, the dissolved carbon dioxide concentration will decrease to its equilibrium value and the beverage will become “flat.”

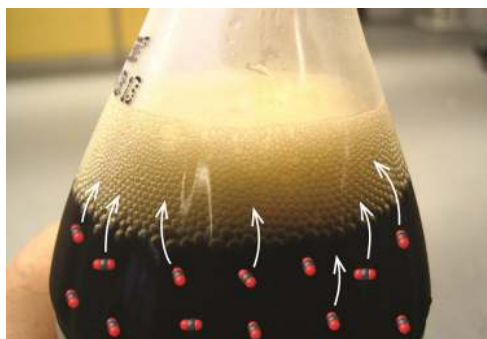


Figure 3.2.1.3: Opening the bottle of carbonated beverage reduces the pressure of the gaseous carbon dioxide above the beverage. The solubility of CO_2 is thus lowered, and some dissolved carbon dioxide may be seen leaving the solution as small gas bubbles. (credit: modification of work by Derrick Coetzee)

A dark brown liquid is shown in a clear, colorless container. A thick layer of beige bubbles appear at the surface of the liquid. In the liquid, thirteen small clusters of single black spheres with two red spheres attached to the left and right are shown. Red spheres represent oxygen atoms and black represent carbon atoms. Seven white arrows point upward in the container from these clusters to the bubble layer at the top of the liquid.

For many gaseous solutes, the relation between solubility, C_g , and partial pressure, P_g , is a proportional one:

$$C_g = kP_g$$

where k is a proportionality constant that depends on the identities of the gaseous solute and solvent, and on the solution temperature. This is a mathematical statement of Henry's law: The quantity of an ideal gas that dissolves in a definite volume of liquid is directly proportional to the pressure of the gas.

✓ Example 3.2.1.1: Application of Henry's Law

At 20 °C, the concentration of dissolved oxygen in water exposed to gaseous oxygen at a partial pressure of 101.3 kPa (760 torr) is $1.38 \times 10^{-3} \text{ mol L}^{-1}$. Use Henry's law to determine the solubility of oxygen when its partial pressure is 20.7 kPa (155 torr), the approximate pressure of oxygen in earth's atmosphere.

Solution

According to Henry's law, for an ideal solution the solubility, C_g , of a gas ($1.38 \times 10^{-3} \text{ mol L}^{-1}$, in this case) is directly proportional to the pressure, P_g , of the undissolved gas above the solution (101.3 kPa, or 760 torr, in this case). Because we know both C_g and P_g , we can rearrange this expression to solve for k .

$$\begin{aligned} C_g &= kP_g \\ k &= \frac{C_g}{P_g} \\ &= \frac{1.38 \times 10^{-3} \text{ mol L}^{-1}}{101.3 \text{ kPa}} \\ &= 1.36 \times 10^{-5} \text{ mol L}^{-1} \text{ kPa}^{-1} \\ &\quad (1.82 \times 10^{-6} \text{ mol L}^{-1} \text{ torr}^{-1}) \end{aligned}$$

Now we can use k to find the solubility at the lower pressure.

$$\begin{aligned} C_g &= kP_g \\ 1.36 \times 10^{-5} \text{ mol L}^{-1} \text{ kPa}^{-1} \times 20.7 \text{ kPa} \\ &\quad (\text{or } 1.82 \times 10^{-6} \text{ mol L}^{-1} \text{ torr}^{-1} \times 155 \text{ torr}) \\ &= 2.82 \times 10^{-4} \text{ mol L}^{-1} \end{aligned}$$

Note that various units may be used to express the quantities involved in these sorts of computations. Any combination of units that yield to the constraints of dimensional analysis are acceptable.

? Exercise 3.2.1.1

Exposing a 100.0 mL sample of water at 0 °C to an atmosphere containing a gaseous solute at 20.26 kPa (152 torr) resulted in the dissolution of 1.45×10^{-3} g of the solute. Use Henry's law to determine the solubility of this gaseous solute when its pressure is 101.3 kPa (760 torr).

Answer

7.25×10^{-3} g in 100.0 mL or 0.0725 g/L

Case Study: Decompression Sickness ("The Bends")

Decompression sickness (DCS), or "the bends," is an effect of the increased pressure of the air inhaled by scuba divers when swimming underwater at considerable depths. In addition to the pressure exerted by the atmosphere, divers are subjected to additional pressure due to the water above them, experiencing an increase of approximately 1 atm for each 10 m of depth. Therefore, the air inhaled by a diver while submerged contains gases at the corresponding higher ambient pressure, and the concentrations of the gases dissolved in the diver's blood are proportionally higher per Henry's law.

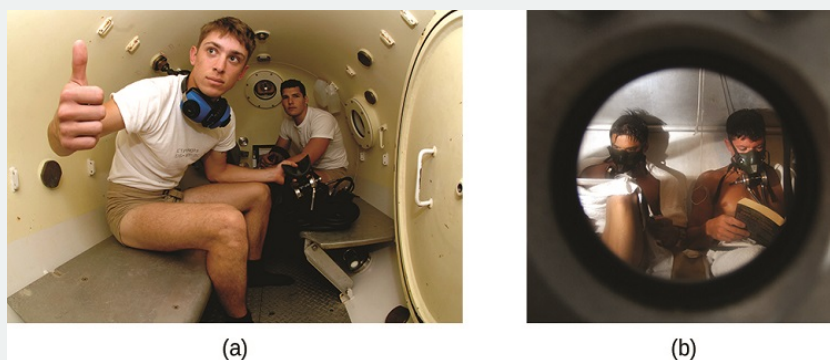
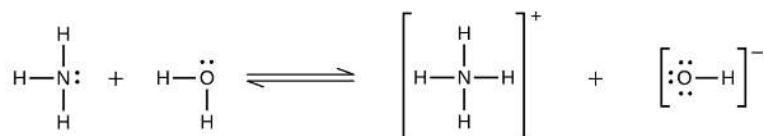


Figure 3.2.1.4: (a) US Navy divers undergo training in a recompression chamber. (b) Divers receive hyperbaric oxygen therapy.

Two photos are shown. The first shows two people seated in a steel chamber on benches that run length of the chamber on each side. The chamber has a couple of small circular windows and an open hatch-type door. One of the two people is giving a thumbs up gesture. The second image provides a view through a small, circular window. Inside the two people can be seen with masks over their mouths and noses. The people appear to be reading.

As the diver ascends to the surface of the water, the ambient pressure decreases and the dissolved gases become less soluble. If the ascent is too rapid, the gases escaping from the diver's blood may form bubbles that can cause a variety of symptoms ranging from rashes and joint pain to paralysis and death. To avoid DCS, divers must ascend from depths at relatively slow speeds (10 or 20 m/min) or otherwise make several decompression stops, pausing for several minutes at given depths during the ascent. When these preventive measures are unsuccessful, divers with DCS are often provided hyperbaric oxygen therapy in pressurized vessels called decompression (or recompression) chambers (Figure 3.2.1.4).

Deviations from Henry's law are observed when a chemical reaction takes place between the gaseous solute and the solvent. Thus, for example, the solubility of ammonia in water does not increase as rapidly with increasing pressure as predicted by the law because ammonia, being a base, reacts to some extent with water to form ammonium ions and hydroxide ions.



Gases can form **supersaturated solutions**. If a solution of a gas in a liquid is prepared either at low temperature or under pressure (or both), then as the solution warms or as the gas pressure is reduced, the solution may become supersaturated. In 1986, more than 1700 people in Cameroon were killed when a cloud of gas, almost certainly carbon dioxide, bubbled from Lake Nyos (Figure 3.2.1.5), a deep lake in a volcanic crater. The water at the bottom of Lake Nyos is saturated with carbon dioxide by volcanic activity beneath the lake. It is believed that the lake underwent a turnover due to gradual heating from below the lake, and the

warmer, less-dense water saturated with carbon dioxide reached the surface. Consequently, tremendous quantities of dissolved CO_2 were released, and the colorless gas, which is denser than air, flowed down the valley below the lake and suffocated humans and animals living in the valley.



Figure 3.2.1.5: (a) It is believed that the 1986 disaster that killed more than 1700 people near Lake Nyos in Cameroon resulted when a large volume of carbon dioxide gas was released from the lake. (b) A CO_2 vent has since been installed to help outgas the lake in a slow, controlled fashion and prevent a similar catastrophe from happening in the future. (credit a: modification of work by Jack Lockwood; credit b: modification of work by Bill Evans)

Two photos are shown. The first is an aerial view of a lake surrounded by green hills. The second shows a large body of water with a fountain sending liquid up into the air several yards or meters above the surface of the water.

Solutions of Liquids in Liquids

We know that some liquids mix with each other in all proportions; in other words, they have infinite mutual solubility and are said to be miscible. Ethanol, sulfuric acid, and ethylene glycol (popular for use as antifreeze, pictured in Figure 3.2.1.6) are examples of liquids that are completely miscible with water. Two-cycle motor oil is miscible with gasoline.



Figure 3.2.1.6: Water and antifreeze are miscible; mixtures of the two are homogeneous in all proportions. (credit: "dno1967"/Wikimedia commons)

Liquids that mix with water in all proportions are usually polar substances or substances that form hydrogen bonds. For such liquids, the dipole-dipole attractions (or hydrogen bonding) of the solute molecules with the solvent molecules are at least as strong as those between molecules in the pure solute or in the pure solvent. Hence, the two kinds of molecules mix easily. Likewise, nonpolar liquids are miscible with each other because there is no appreciable difference in the strengths of solute-solute, solvent-solvent, and solute-solvent intermolecular attractions. The solubility of polar molecules in polar solvents and of nonpolar molecules in nonpolar solvents is, again, an illustration of the chemical axiom "like dissolves like."

Two liquids that do not mix to an appreciable extent are called immiscible. Layers are formed when we pour immiscible liquids into the same container. Gasoline, oil (Figure 3.2.1.7), benzene, carbon tetrachloride, some paints, and many other nonpolar liquids are immiscible with water. The attraction between the molecules of such nonpolar liquids and polar water molecules is ineffectively weak. The only strong attractions in such a mixture are between the water molecules, so they effectively squeeze out the molecules of the nonpolar liquid. The distinction between immiscibility and miscibility is really one of degrees, so that miscible liquids are of infinite mutual solubility, while liquids said to be immiscible are of very low (though not zero) mutual solubility.



Figure 3.2.1.7: Water and oil are immiscible. Mixtures of these two substances will form two separate layers with the less dense oil floating on top of the water. (credit: "Yortw"/Flickr)

This is a photo of a clear, colorless martini glass containing a golden colored liquid layer resting on top of a clear, colorless liquid.

Two liquids, such as bromine and water, that are of moderate mutual solubility are said to be partially miscible. Two partially miscible liquids usually form two layers when mixed. In the case of the bromine and water mixture, the upper layer is water, saturated with bromine, and the lower layer is bromine saturated with water. Since bromine is nonpolar, and, thus, not very soluble in water, the water layer is only slightly discolored by the bright orange bromine dissolved in it. Since the solubility of water in bromine is very low, there is no noticeable effect on the dark color of the bromine layer (Figure 3.2.1.8).



Figure 3.2.1.8: Bromine (the deep orange liquid on the left) and water (the clear liquid in the middle) are partially miscible. The top layer in the mixture on the right is a saturated solution of bromine in water; the bottom layer is a saturated solution of water in bromine. (credit: Paul Flowers)

This figure shows three test tubes. The first test tube holds a dark orange-brown substance. The second test tube holds a clear substance. The amount of substance in both test tubes is the same. The third test tube holds a dark orange-brown substance on the bottom with a lighter orange substance on top. The amount of substance in the third test tube is almost double of the first two.

Solutions of Solids in Liquids

The dependence of solubility on temperature for a number of inorganic solids in water is shown by the solubility curves in Figure 3.2.1.9. Reviewing these data indicate a general trend of increasing solubility with temperature, although there are exceptions, as illustrated by the ionic compound cerium sulfate.

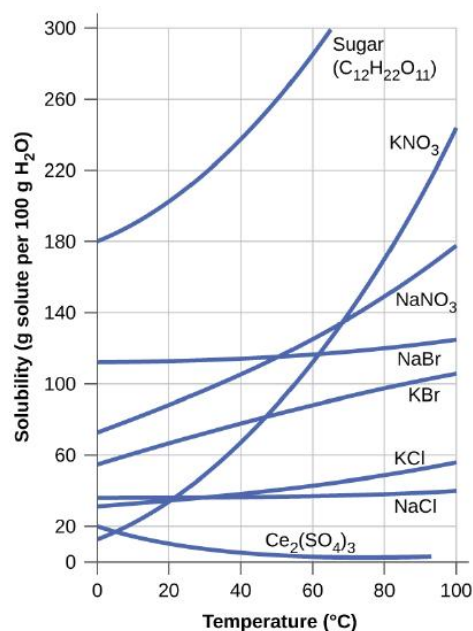


Figure 3.2.1.9: This graph shows how the solubility of several solids changes with temperature.

This shows a graph of the solubility of sugar C subscript 12 H subscript 22 O subscript 11, K N O subscript 3, N a N O subscript 3, N a B r, K B r, N a subscript 2 S O subscript 4, K C l, and C e subscript 2 left parenthesis S O subscript 4 right parenthesis subscript 3 in g solute per 100 g H subscript 2 O at temperatures ranging from 0 degrees Celsius to 100 degrees Celsius. At 0 degrees Celsius, solubilities are approximately 180 for sugar C subscript 12 H subscript 22 O subscript 11, 115 for K N O subscript 3, 75 for N a N O subscript 3, 115 for N a B r, 55 for K B r, 7 for N a subscript 2 S O subscript 4, 25 for K C l, and 20 for C e subscript 2 left parenthesis S O subscript 4 right parenthesis subscript 3. At 100 degrees Celsius, sugar C subscript 12 H subscript 22 O subscript 11 has exceeded the upper limit of solubility indicated on the graph, 240 for K N O subscript 3, 178 for N a N O subscript 3, 123 for N a B r, 105 for K B r, 52 for N a subscript 2 S O subscript 4, 58 for K C l, and the graph for C e subscript 2 left parenthesis S O subscript 4 right parenthesis subscript 3 stops at about 92 degrees Celsius where the solubility is nearly zero. The graph for N a subscript 2 S O subscript 4 is shown in red. All others substances are shown in blue. The solubility of this substance increases until about 30 degrees Celsius and declines beyond that point with increasing temperature.

The temperature dependence of solubility can be exploited to prepare supersaturated solutions of certain compounds. A solution may be saturated with the compound at an elevated temperature (where the solute is more soluble) and subsequently cooled to a lower temperature without precipitating the solute. The resultant solution contains solute at a concentration greater than its equilibrium solubility at the lower temperature (i.e., it is supersaturated) and is relatively stable. Precipitation of the excess solute can be initiated by adding a seed crystal (see the video in the Link to Learning earlier in this module) or by mechanically agitating the solution. Some hand warmers, such as the one pictured in Figure 3.2.1.10 take advantage of this behavior.



Figure 3.2.1.10: This hand warmer produces heat when the sodium acetate in a supersaturated solution precipitates. Precipitation of the solute is initiated by a mechanical shockwave generated when the flexible metal disk within the solution is “clicked.” (credit: modification of work by “Velela”/Wikimedia Commons)

Three photos of hand warmers are shown side by side with an arrow pointing from the first photo to the second, and another arrow pointing from the second photo to the third. The first packet contains a clear colorless liquid and a small metal disc can be seen. In the second packet, the disc can't be seen and a dispersion of white liquid is beginning. In the third packet, all of the liquid is white.



Video 3.2.1.2 This video shows the crystallization process occurring in a hand warmer.

Summary

The extent to which one substance will dissolve in another is determined by several factors, including the types and relative strengths of intermolecular attractive forces that may exist between the substances' atoms, ions, or molecules. This tendency to dissolve is quantified as substance's solubility, its maximum concentration in a solution at equilibrium under specified conditions. A saturated solution contains solute at a concentration equal to its solubility. A supersaturated solution is one in which a solute's concentration exceeds its solubility—a nonequilibrium (unstable) condition that will result in solute precipitation when the solution is appropriately perturbed. Miscible liquids are soluble in all proportions, and immiscible liquids exhibit very low mutual solubility. Solubilities for gaseous solutes decrease with increasing temperature, while those for most, but not all, solid solutes increase with temperature. The concentration of a gaseous solute in a solution is proportional to the partial pressure of the gas to which the solution is exposed, a relation known as Henry's law.

Key Equations

- $C_g = kP_g$

Glossary

Henry's law

law stating the proportional relationship between the concentration of dissolved gas in a solution and the partial pressure of the gas in contact with the solution

immiscible

of negligible mutual solubility; typically refers to liquid substances

miscible

mutually soluble in all proportions; typically refers to liquid substances

partially miscible

of moderate mutual solubility; typically refers to liquid substances

saturated

of concentration equal to solubility; containing the maximum concentration of solute possible for a given temperature and pressure

solubility

extent to which a solute may be dissolved in water, or any solvent

supersaturated

of concentration that exceeds solubility; a nonequilibrium state

unsaturated

of concentration less than solubility

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3.2.2: Overview of Chromatography

The first uses of chromatography involved separating the colored components of plants in the early 1900's. The pigments in a plant can be separated into yellow, orange and green colors (xanthophylls, carotenes and chlorophylls respectively) through this method. The Greek name for color is *chroma*, and *graphein* is 'to write,' so chromatography can be thought of as "color writing."

The general idea of chromatography can be demonstrated with food dyes in your kitchen. Commercial green food dye does not contain any green colored components at all, and chromatography can show that green food dye is actually a mixture of blue and yellow dyes. If a drop of green food dye is placed in the middle of a paper towel followed by a few drops of water, the water will creep outwards as it wets the paper (Figure 2.1). As the water expands, the dye will travel with it. If you let the dye expand long enough, you'll see that the edges will be tinted with blue (Figure 2.1d). This is the beginning of the separation of the blue and yellow components in the green dye by the paper and water.

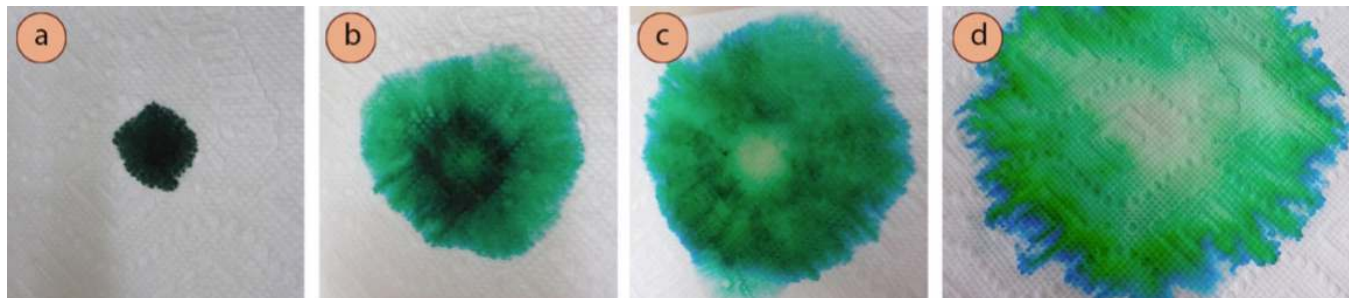


Figure 2.1: Time-lapse sequence of a drop of green food dye on a paper towel, followed by a drop of water.

A complete separation of the green food dye can be accomplished using paper chromatography. A dilute sample is deposited on the bottom edge of a piece of paper, the paper is rolled in a cylinder, stapled, and placed vertically in a closed container containing a small amount of solvent¹ (Figure 2.2a). The solvent is allowed to wick up the paper through capillary action (called "elution," Figure 2.2b), and through this method complete separation of the blue and yellow components can be achieved (Figure 2.2d).

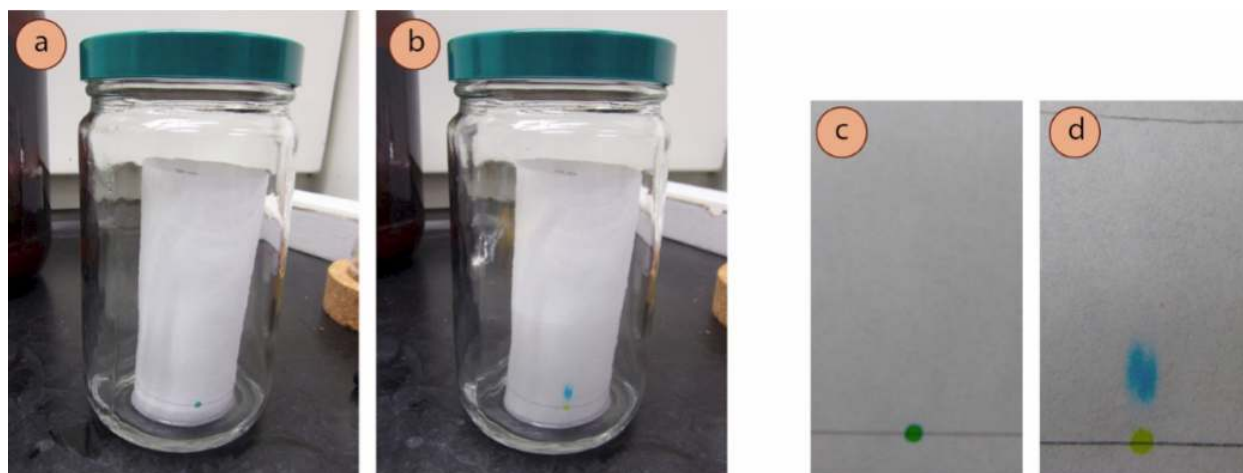


Figure 2.2: Paper chromatography of diluted green food dye: a) Before elution, b) After elution, c) Zoom in before elution, d) Zoom in after elution.

¹The solvent used in this separation is a solution made from a 1:3:1 volume ratio of 6 M NH_4OH :1-pentanol:ethanol.

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3.3: Separating Mixtures of Liquids

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3.3.1: Uses of Simple Distillation

Concentration of Alcohol

Fermented grains can produce a maximum alcohol content of about 16%, the upper limit of most beers and wines, as the yeast organism used in fermentation cannot survive in more concentrated alcoholic solutions. However, spirits such as gin, vodka, and rum usually have an alcohol content of roughly 40% by volume. Distillation is the method used to concentrate fermented solutions and produce hard liquors. A distillation of fermented grape juice is commonly done in academic laboratories (Figure 5.2).



Figure 5.2: Distillation of fermented grape juice during a lab at Butte College.

Figure 5.3 shows the distillation of red wine. Notice how the wine is noticeably purified in the process as the distillate is clear (Figure 5.3d). All concentrated alcoholic products at first distill clear, but some become colored during the aging process (from components leaching out of the barrels they are stored in, or from oxidation).

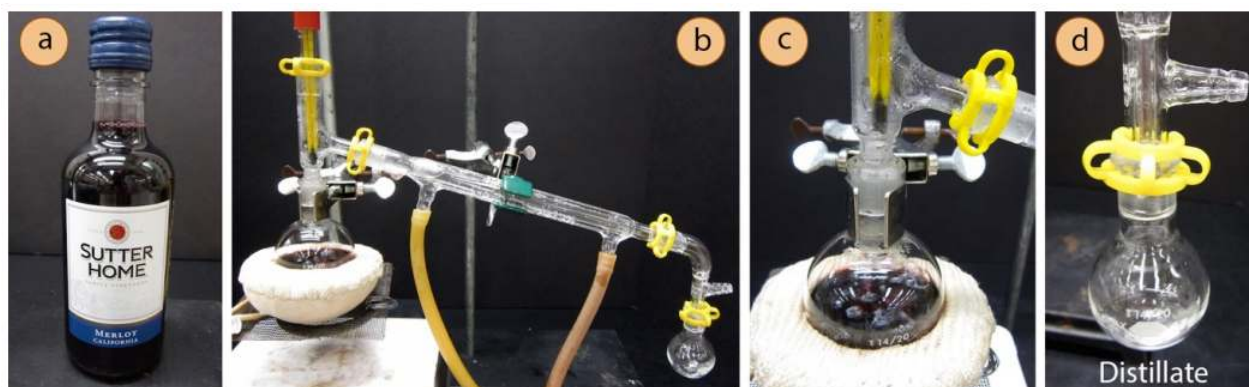


Figure 5.3: a) Red wine, b) Distillation of red wine, c) Distilling flask during the process, d) Distillate (brandy).

The distillation of red wine can be proven to have concentrated the alcohol through a flame test, which is the origin of the term "proof". In the 16th century when rum was a bartering item, it was regularly tested to ensure that it had not been watered down. An alcoholic sample that is 57% alcohol by volume is capable of catching on fire, while more dilute solutions cannot, enabling ignition to serve as "proof" of alcohol content. The red wine used in Figure 5.3 did not ignite, which is consistent with its label that states it to be only 13% alcohol (Figure 5.4a). The distillate easily caught on fire (Figure 5.4c+d), and density analysis showed it to be 67% alcohol.

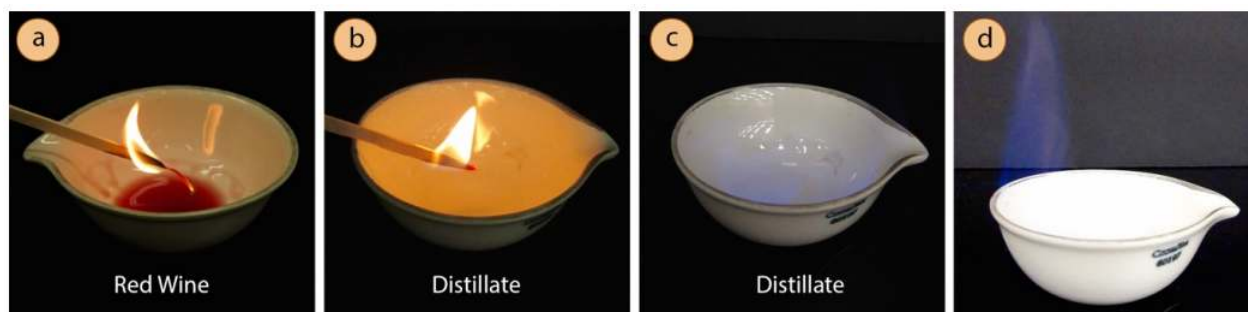


Figure 5.4: a) Unsuccessful ignition of red wine, b) Successful ignition of the distillate, c+d) The distillate aflame (faint blue).

Distilled Water

Access to clean, fresh water is a major problem facing the world today. In countries neighboring the ocean, seawater desalination is sometimes used to provide the country with drinkable water. Distillation is one of the main methods¹ used to purify ocean water and works well since salt, microorganisms, and other components of seawater are non-volatile. The main disadvantage of distilling water is that the process requires a lot of energy, and unless engineered creatively, the economics can be a major deterrent to using the method. Heat released from a power plant is often used to provide the energy for the distillation of seawater, and Saudi Arabia and Israel mainly use coupled power plants and distilleries to obtain roughly half the fresh water needed for their countries.²

Along with drinking water, distilled water is necessary for scientific lab work as dissolved salts in tap water may interfere with some experiments. Many science buildings have their own distilled water generators (Figure 5.5a), enabling wash bottles and carboys to be filled with a turn of the spigot (Figure 5.5b).



Figure 5.5: a) Distilled water generator at Butte College. The top metallic box is the actual generator, and the bottom cylindrical container is the reservoir, b) Distilled water carboy and wash bottle.

Purification of Reagents and Products

Distillation is an excellent purification tool for many liquids, and can be used to purify products from a chemical reaction. Figure 5.6 shows the distillation of a crude sample of isoamyl acetate, formed through a Fischer esterification reaction. The crude sample was originally yellow (Figure 5.6a), but the distillate was colorless (Figure 5.6d), making obvious the removal of some materials through the process.

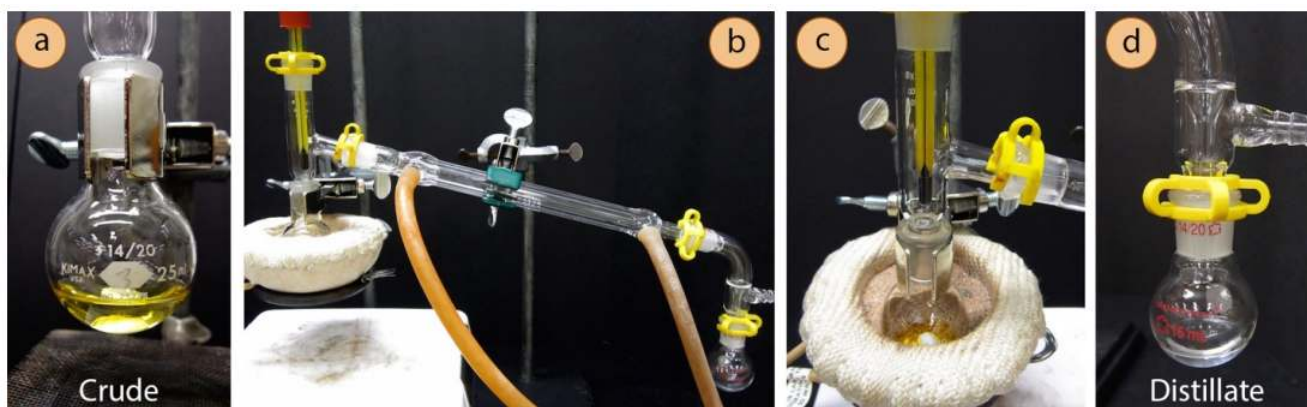


Figure 5.6: a) Crude yellow isoamyl acetate formed from a Fischer esterification, b+c) Simple distillation, d) Colorless distillate.

Distillation can also be used to purify reagents that have degraded over time. Figure 5.7a shows a bottle of benzaldehyde that has partially oxidized, as evidenced by the crystals of benzoic acid seen adhering to the inside of the glass (indicated with an arrow). A simple distillation purified the benzaldehyde sample, and its effectiveness was demonstrated through comparison of the infrared (IR) spectra of the original material (Figure 5.8a) and the distillate (Figure 5.8b). The broad region indicated by an arrow in Figure 5.8a represent the O–H stretch of a carboxylic acid (benzoic acid), and the distillate's IR spectrum lacks this feature.



Figure 5.7: a) Benzaldehyde reagent with crystals of benzoic acid seen on the glassware (indicated with an arrow), b+c) Distillation.

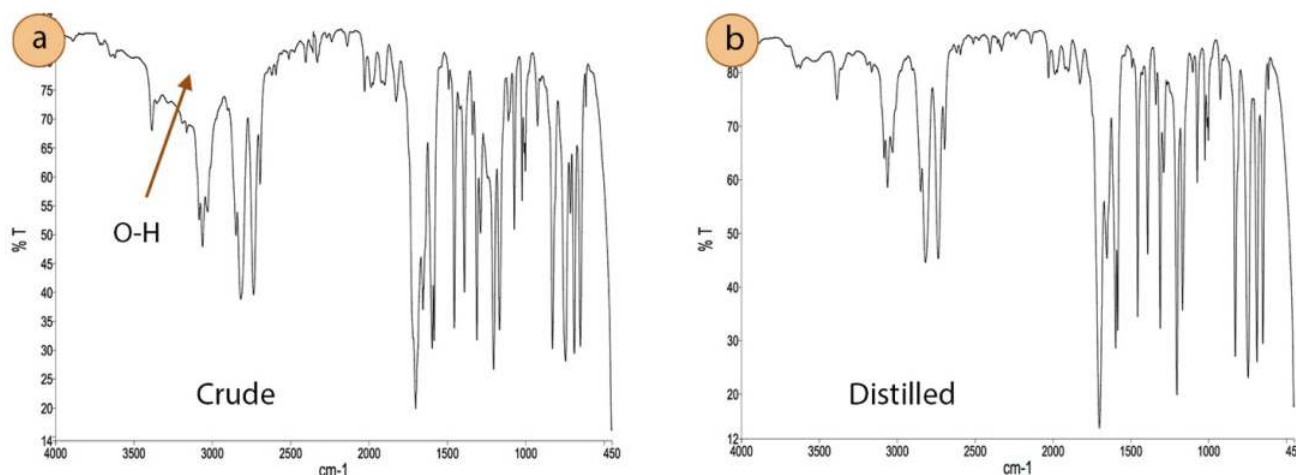


Figure 5.8: a) IR spectrum of benzaldehyde before distillation (arrow points to the O–H signal from the benzoic acid impurity), b) IR spectrum of benzaldehyde after distillation.

¹More often, vacuum distillation is used for desalination, as the lowered pressure allows for boiling to occur at a lower temperature (which requires less energy). Vacuum distillation of seawater is still energy intensive. Reverse osmosis is also used for seawater desalination.

²Pyper, Julia, "Israel is creating a water surplus using desalination," *E+E News*, February 7, 2014.

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3.4: Detoxification

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3.4.1: Sanitation of Drinking Water

Learning Objectives

- Understand why drinking water required sanitation.
- Know the three different types of water sanitation methods.
- Provide advantages and disadvantages of each type of sanitation method.
- Define the terms residual protection and disinfection byproducts.

Chlorine-based methods

Chlorination is the process of adding chlorine compounds to drinking water to disinfect it and kill germs. In 1908, New Jersey was the first state to utilize chlorinated compounds for sanitizing drinking water. This method is quite cheap for most countries and rids water of bacteria and most viruses. Regarding protozoa (*Giardia* and *Cryptosporidium*), results can vary depending upon the type of chlorine product that it used and how long it is applied (refer to this CDC table). Chlorine does offer residual protection from treatment facility to consumer and is quite cheap. In the United States, chlorine (Cl_2) has been used to sanitize both drinking and waste waters since the early twentieth century. Gaseous chlorine (Cl_2) is known to be quite corrosive, poisonous, and explosive.



Video 3.4.1.1: Chlorine and Exposure Concerns. (Copyright; <https://www.youtube.com/@IAQMarketer>). (3:45min)

After watching the video above, answer the questions below:

- 1) Provide the physical and chemical properties of chlorine (Cl_2).
- 2) When was chlorine gas used as a chemical weapon?
- 3) What are some biological reactions to chlorine gas exposure?
- 4) Name the two household cleaners that should never be mixed together.

Other chlorine-based sanitizing agents include chlorine dioxide (ClO_2), sodium hypochlorite (NaClO), calcium hypochlorite ($\text{Ca}(\text{ClO})_2$), and chloroamines (e.g., NH_2Cl). The first of these, chlorine dioxide, is a gaseous compound that is capable of destroying viruses and bacteria in drinking water, but requires higher dosages to kill protozoa like *Giardia*. Sanitizing procedures involving chlorine dioxide require longer contact time at higher dosages than other using pure chlorine. Hypochlorite (ClO^-) based compounds are effective at killing viruses and bacteria. Like chlorine dioxide, hypochlorites do not deactivate all protozoa. Deactivating *Cryptosporidium* can be challenging using chlorine based methods. In order to remove this protozoa, water must be flushed through a filter which has a pore size of equal to or less than 1 micron (micrometer). Filters should be labeled as "absolute 1 micron." If reverse osmosis is used to purify water, *Cryptosporidium* and all other disease causing pathogens will be removed as well.



Figure 3.4.1.1: Image of chlorine dioxide dissolved in water. (Copyright, <https://commons.wikimedia.org/wiki/User:Iridos>)

Chloroamines are a group of chemical compounds that contain chlorine (Cl_2) and ammonia (NH_3). The specific form of chloroamine used in drinking water disinfection is called monochloramine (NH_2Cl). These sanitizers do not kill harmful organisms as fast as chlorine gas and can decompose when exposed to heat, light, and bacteria. Effective chloramine levels range from 1.0 to 4.0 ppm. These compounds provide long-lasting residual protection. For this reason, monochloramine is often utilized as a secondary sanitizer in addition to chlorine or non-chlorine methods of sanitization.

All forms of chlorination do alter smell and taste of drinking water. In addition, chlorine (most often responsible are the chloroamines compounds) can react with other chemicals in tap water to produce organochlorides. The EPA classifies these newly formed compounds as disinfectant byproducts and regulates them as primary drinking water contaminants.

Ozone (O_3) Disinfection

Ozone disinfection, or ozonation, is a powerful oxidizing process which is toxic to most waterborne organisms. This method of disinfection is widely used in Europe. Ozone deactivates cyst formation of protozoa (like *Giardia*). In addition, this chemical effectively kills viruses and bacteria.

Ozone machines were first constructed in the mid-1800's. New devices produce O_3 molecules by passing oxygen through ultraviolet light or a "cold" electrical discharge. To use ozone as a disinfectant, it must be created on-site and then added to the water by bubble contact. Unlike chlorine, the ozonation process does not alter the taste or smell of water.



Video 3.4.1.2 Demonstration-Effects of Panasonic's "Ozone Water" Device (1.11 min).

Unfortunately, ozone does not provide any residual protection once water has left the treatment facility. For water that must travel far distances to consumers, chlorine or chloramine should be added throughout a distribution system to remove any potential pathogens during the transportation process.

However, although fewer by-products are formed by ozonation, it has been discovered that ozone reacts with bromide ions in water to produce concentrations of a suspected carcinogen called bromate (BrO_3)¹⁻. Bromide (Br^-) can be found in fresh water supplies in sufficient concentrations to produce (after ozonation) more than 10 parts per billion (ppb) of bromate — the maximum contaminant level established by the EPA. Other disadvantages to using ozonation methods are energy requirements and cost. Of the three types of sanitization processes (chlorination, ozonation, and UV irradiation), this technique is the most expensive.

Ultraviolet Disinfection (UV)

Ultraviolet radiation (namely UVC) can be used to eradicate viruses, bacteria, and parasites from drinking water. This method of sanitation does not produce byproducts or alter physical properties (taste or smell) of the water.



Video 3.4.1.3 Understanding Ultraviolet UV Radiation and its Effects. (Copyright, Larson Electronics). (1:54 min).

However, ionizing radiation has difficulty inactivating parasitic cysts in turbid (unclear) water. Like ozonation, UV irradiation offers no residual protection and is pricier than chlorination. Smaller ultraviolet units do supply over 2 million people in 28 developing countries clean water for drinking, eating, and cooking.



Figure 3.4.1.2 Ultraviolet lamp sanitizing water. Image courtesy of: <https://www.nab.usace.army.mil/Media/News-Stories/Article/946068/army-water-treatment-plant-brings-a-unique-first/>

References

- 1) <https://www.oxidationtech.com/ozone/history.html>
- 2) 14.6: Making Water Fit to Drink - Chemistry LibreTexts
- 3) https://r.search.yahoo.com/_ylt=Awri...6JpE5SOBYtIBC-
- 4) [cdc.gov](https://www.cdc.gov)

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3.4.2: Other Water treatment processes

Learning Objectives

- Objective 1
- Objective 2

Drinking Water Treatment

The process of water treatment to provide safe drinking water for their communities. There are various combinations and types of processes in water treatment depending on the scale of the plant and quality of the raw (source) water. Today, the most common steps in water treatment used by community water systems (mainly surface water treatment).



Figure 3.4.2.1: Dirty water spilling out of a large glass carboy on its side.(CC-SA-3.0, Ildar Sagdejev, Wikipedia Commons)

Coagulation and Flocculation

Before these processes, raw water is run through a screen to separate visible solids from the liquid. Next, Aluminum sulfate $\text{Al}_2(\text{SO}_4)_3$ and Calcium hydroxide $\text{Ca}(\text{OH})_2$ are added to the liquid. The aluminum based compound is often called alum and induces clumping of suspended particules. This process is called flocculation. Calcium hydroxide (also known as lime) raises the pH of the mixture and produces more charged species (electrolytes) on the suspended particles. These charges are extracted and increase the size of the solid (coagulate) which simplify the filtration process.



The slightly basic water causes $\text{Al}(\text{OH})_3$, $\text{Fe}(\text{OH})_3$ and $\text{Fe}(\text{OH})_2$ to precipitate, bringing the small particulates with them and the water becomes clear. Some records have been found that Egyptians and Romans used these techniques as early as 2000 BC.

Suspension of iron oxide particulates and humic organic matter in water gives water the yellow muddy appearance. Both iron oxide particulates and organic matter can be removed from coagulation and flocculation. The description given here is oversimplified, and many more techniques have been applied in the treatment of water. Coagulation is a major application of lime in the treatment of wastewater.

Other salts such as iron sulfates $\text{Fe}_2(\text{SO}_4)_3$ and FeSO_4 , chromium sulfate $\text{Cr}_2(\text{SO}_4)_3$, and some special polymers are also useful. Other ions such as sodium, chloride, calcium, magnesium, and potassium also affect the coagulation process. So do temperature, pH, and concentration.

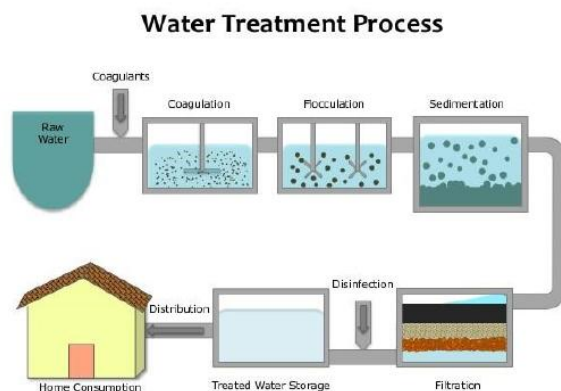


Figure 3.4.2.2: A diagram showing the process of water purification. (CC-SA-4.0; <https://dreamcivil.com/water-treatment-process/>)

Sedimentation

During sedimentation, floc settles to the bottom of the water supply, due to its weight. This settling process is called sedimentation. The floc particles are then removed from the bottom of the basins.

Aeration

Bringing air into intimate contact with water for the purpose of exchanging certain components between the two phases is called **aeration**. Oxygenation is one of the purposes of aeration. Others are removal of volatile organic substances, hydrogen sulfide, ammonia, and volatile organic compounds



Figure 3.4.2.3: Furman University Library (James B. Duke Library) and fountains. (Copyright; https://commons.wikimedia.org/w/index.php?title=Furman_University_Library&redlink=1)

Filtration

Once the floc has settled to the bottom of the water supply, the clear water on top will pass through filters of varying compositions (sand, gravel, and charcoal) and pore sizes, in order to remove dissolved particles, such as dust, parasites, bacteria, viruses, and chemicals.

Sanitization

After the water has been filtered, a chemical disinfectant (chlorine and/or ozone based) or ultraviolet radiation will be applied in order to kill any remaining parasites, bacteria, and viruses, and to protect the water from germs when it is piped to homes and businesses.

Fluoridation

This process is not mandatory for water processing plants in the United States. Around 72% of public water systems have this chemical added in order to reduce dental issues.

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- [Chung \(Peter\) Chieh](#) (Professor Emeritus, Chemistry @ University of Waterloo)

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CHAPTER OVERVIEW

4: Designing Drugs

4.1: Drug Design

4.2: How Drugs Work

4.2.1: Pain Relievers- From Aspirin to Oxycodone

4.2.2: Cold and Allergy Medicines

4.3: Pharmacokinetics

4.4: Drugs vs. Poisons- All About the Dose

4.4.1: Natural Poisons and Food Poisoning

4.4.2: The Lethal Dose

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4.1: Drug Design

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4.2: How Drugs Work

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4.2.1: Pain Relievers- From Aspirin to Oxycodone

Learning Objectives

- Know the difference between anti-inflammatory, analgesic and antipyretic drugs.
- Describe how aspirin and other NSAIDs work.
- Know the side effects of taking prescription and non-prescription medications
- Know the risks of addiction, abuse, and overdose of prescription opioids.

A **drug** is any substance that causes a change in an organism's physiology or psychology when consumed. Drugs are typically distinguished from food and substances that provide nutritional support. Consumption of drugs can be via inhalation, injection, smoking, ingestion, absorption via a patch on the skin, suppository, or dissolution under the tongue.

Anti-inflammatory, analgesic (pain reliever or pain killer), and antipyretic (fever reducer) drugs are a heterogeneous group of compounds, often chemically unrelated (although most of them are organic acids), which nevertheless share certain therapeutic actions and side effects. The prototype is aspirin; hence these compounds are often referred to as aspirin-like drugs. All aspirin-like drugs are antipyretic, analgesic, and anti-inflammatory, but there are important differences in their activities. For example, acetaminophen is antipyretic and analgesic but is only weakly anti-inflammatory. The reason for the differences are not clear; variations in the sensitivity of enzymes in the target tissues may be important.

When employed as analgesics, these drugs are usually effective only against pain of low-to-moderate intensity, particularly that associated with inflammation. Aspirin drugs do not change the perception of sensory modalities other than pain. The type of pain is important; chronic postoperative pain or pain arising from inflammation is particularly well controlled by aspirin-like drugs, whereas pain arising from the hollow viscera is usually not relieved.

Over-the-counter (OTC) medicines are good for many types of pain. There are two main types of OTC pain medicines: acetaminophen (Tylenol) and nonsteroidal anti-inflammatory drugs (NSAIDs). Aspirin, naproxen (Aleve), and ibuprofen (Advil, Motrin) are examples of OTC NSAIDs.

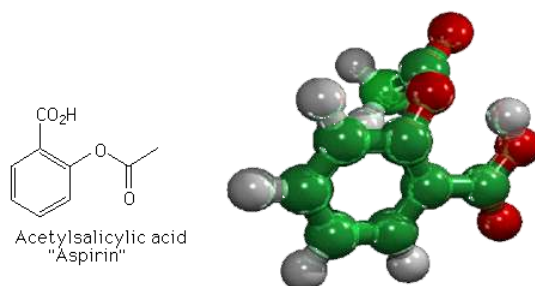
If OTC medicines don't relieve one's pain, the doctor may prescribe something stronger. Many NSAIDs are also available at higher prescription doses. The most powerful pain relievers are **opioids**. They are very effective, but they can sometimes have serious side effects. There is also a risk of **addiction**. Because of the risks, you must use them only under a doctor's supervision.

Aspirin and other NSAIDs

Nonsteroidal anti-inflammatory drugs (NSAIDs) are members of a drug class that reduces pain, decreases fever, prevents blood clots, and in higher doses, decreases inflammation. Side effects depend on the specific drug but largely include an increased risk of gastrointestinal ulcers and bleeds, heart attack, and kidney disease.

The term *nonsteroidal* distinguishes these drugs from steroids, which while having a similar eicosanoid-depressing, anti-inflammatory action, have a broad range of other effects. First used in 1960, the term served to distance these medications from steroids, which were particularly stigmatised at the time due to the connotations with anabolic steroid abuse. The most prominent NSAIDs are aspirin, ibuprofen, and naproxen, all available over the counter (OTC) in most countries.

In the U.S., about 10 to 20 thousand tons of **aspirin** are consumed each year; it is our most popular analgesic. Aspirin is one of the most effective analgesic, antipyretic, and anti-inflammatory agents.



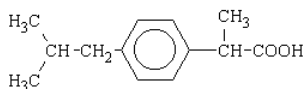
Chemical structure

Figure 4.2.1.1 Aspirin

Aspirin is known to interfere with the action of the platelets. As a result, some people who take a lot of aspirin experience easy bruising of the skin. Therefore, people who have major bleeding problems should not take aspirin. Also, keep in mind that aspirin should not be taken for 10-14 days before surgery (including surgery in the mouth) to avoid excessive bleeding during or after the operation. These side effects probably depend on aspirin-like drugs' ability to block endogenous prostaglandin biosynthesis. Platelet function appears to be disturbed because aspirin-like drugs prevent the formation by the platelets of thromboxane A₂ (TXA₂), a potent aggregating agent. This accounts for the tendency of these drugs to increase the bleeding time.

Other Aspirin-Like Drugs

There are other non-selective NSAIDs on the market, including diclofenac, ibuprofen, ketoprofen, meloxicam, naproxen, and oxaprozin. Ibuprofen and naproxen are available in both prescription and over-the-counter (OTC) versions. The doses in OTC ibuprofen (Advil and Motrin) or naproxen (Aleve) are about half the doses of prescription versions.



Ibuprofen

Figure 4.2.1.2 Ibuprofen.

How NSAIDs Work?

Non-selective NSAIDs like aspirin work (Figure 4.2.1.3) by inhibiting two enzymes that are involved with pain and inflammation —cyclooxygenase-1 and cyclooxygenase-2 (COX-1 and COX-2). These enzymes are involved with the ring closure and addition of oxygen to arachidonic acid converting to prostaglandins. The acetyl group on aspirin is hydrolyzed and then bonded to the alcohol group of serine as an ester (Figure 4.2.1.2). This has the effect of blocking the channel in the enzyme and arachidonic acid can not enter the active site of the enzyme. By inhibiting or blocking this enzyme, the synthesis of prostaglandins is blocked, which in turn relieves some of the effects of pain and fever. Aspirin is also thought to inhibit the prostaglandin synthesis involved with unwanted blood clotting in coronary heart disease. At the same time an injury while taking aspirin may cause more extensive bleeding.

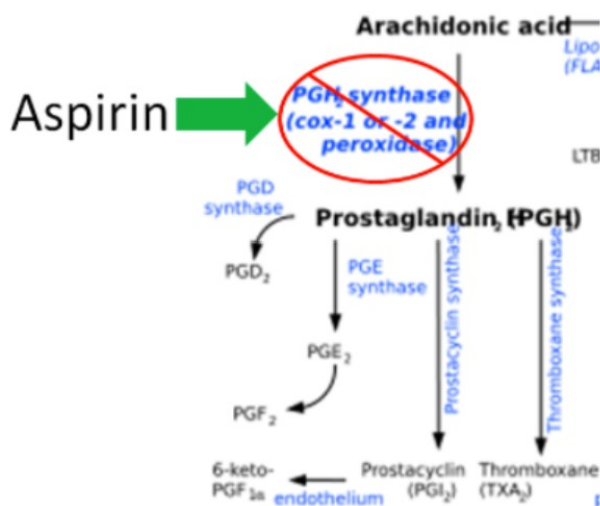


Figure 4.2.1.3 Aspirin inhibition of COX-1 and COX-2 enzymes.

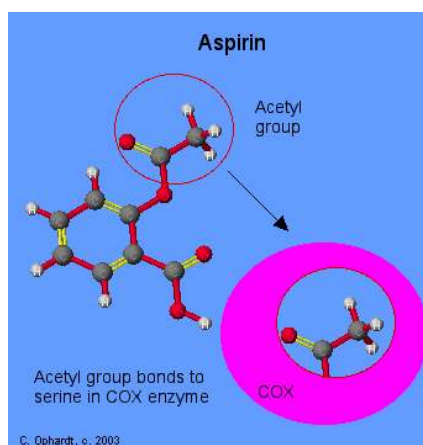


Figure 4.2.1.4 The acetyl group (from aspirin) bonds to serine in COX enzyme.

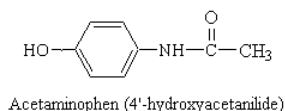
COX-2 selective inhibitors are a newer type of medicine that block the COX-2 enzyme more than the COX-1 enzyme. The only COX-2 selective inhibitor currently on the market in the United States is the prescription drug Celebrex (celecoxib), which is marketed by Pfizer. It was believed that COX-2 inhibitors may be less likely to cause the stomach problems associated with the older NSAIDs, but all NSAIDs carry the risk of stomach problems.

Key Points to Remember With NSAIDs

- Too much can cause stomach bleeding. This risk increases in people who are over 60 years of age, are taking prescription blood thinners, are taking steroids, have a history of stomach bleeding or ulcers, and/or have other bleeding problems.
- Use of NSAIDs can also cause kidney damage. This risk may increase in people who are over 60 years of age, are taking a diuretic (a drug that increases the excretion of urine), have high blood pressure, heart disease, or pre-existing kidney disease.

Acetaminophen

Acetaminophen is an effective alternative to aspirin as an analgesic and antipyretic agent. However, its anti-inflammatory effect is minor and not clinically useful. It is commonly felt that acetaminophen may have fewer side effects than aspirin, but it should be noted that an acute overdose may produce severe or even fatal liver damage. Acetaminophen does not inhibit platelet aggregation and therefore is not useful for preventing vascular clotting.



Side effects are usually fewer than those of aspirin; the drug produces less gastric distress and less ringing in the ears. However, as stated previously, overdose can lead to severe damage of the liver.

Acetaminophen has been proved to be a reasonable substitute for aspirin when analgesic or antipyretic effectiveness is desired, especially in patients who cannot tolerate aspirin. This might include patients with peptic ulcer disease or gastric distress or those in whom the anticoagulant action of aspirin might be undesirable.

Key Points to Remember With Acetaminophen

- Taking a higher dose than recommended will not provide more relief and can be dangerous.
- Too much can lead to liver damage and death. Risk for liver damage may be increased in people who drink three or more alcoholic beverages a day while using acetaminophen-containing medicines.
- Be cautious when giving acetaminophen to children. Infant drop medications can be significantly stronger than regular children's medications. Read and follow the directions on the label every time you use a medicine. Be sure that your infant is getting the infants' pain formula and your older child is getting the children's pain formula.

Prescription Medications

Typical prescription pain relief medicines include opioids and non-opioid medications. Types of prescription opioid medications (Figures 4.2.1.6 and 4.2.1.7) include:

- **morphine**, which is often used before and after surgical procedures to alleviate severe pain
- **oxycodone**, which is also often prescribed for moderate to severe pain
- **codeine**, which comes in combination with acetaminophen or other non-opioid pain relief medications and is often prescribed for mild to moderate pain
- **hydrocodone**, which comes in combination with acetaminophen or other non-opioid pain relief medications and is prescribed for moderate to moderately severe pain

Derived from opium, opioid drugs are very powerful products. They act by attaching to a specific "receptor" in the brain, spinal cord, and gastrointestinal tract. Opioids can change the way a person experiences pain. The term opium refers to the crude resinous extract obtained from the opium poppy. Crude opium contains a wide variety of ingredients, including morphine and codeine, both of which are widely used in medicine. The bulk of the ingredients of opium, however, consists of such organic substances as resins, oils, sugars, and proteins that account for more than 75 % of the weight of the opium but exert little pharmacological activity. Morphine is the major pain relieving drug found in opium, being approximately 10% of the crude exudate. Codeine is structurally close to morphine (see Figure 4.2.1.6), although it is much less potent and amounts to only 0.5% of the opium extract. Heroin does not occur naturally but is a semisynthetic derivative produced by a chemical modification of morphine that increases the potency. It takes only 3 mg. of heroin to produce the same analgesic effect as 10 mg of morphine. However, at these equally effective doses, it may be difficult to distinguish between the effects of the two compounds.

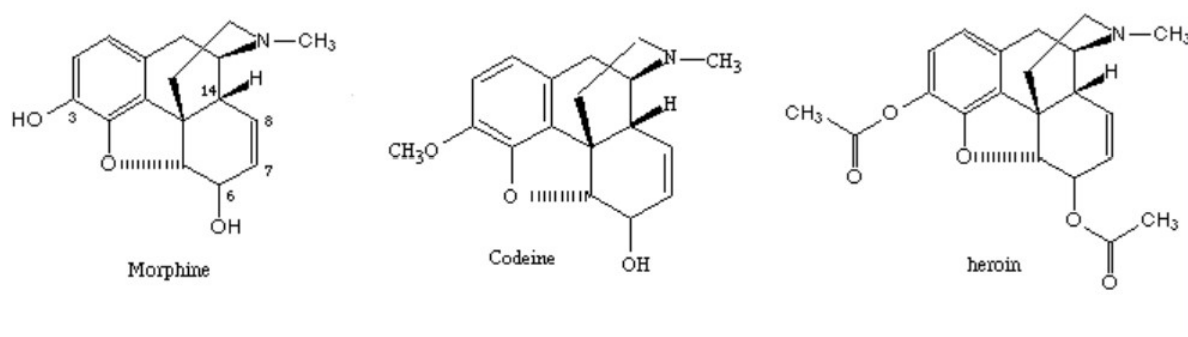


Figure 4.2.1.6 Morphine, codeine and heroin.

Oxycodone and hydrocodone are used to relieve moderate to severe pain. Oxycodone and hydrocodone extended-release tablets and extended-release capsules are used to relieve severe pain in people who are expected to need pain medication around the clock for a long time and who cannot be treated with other medications.

Addiction and Overdose

Anyone who takes prescription opioids can become addicted to them. In fact, as many as one in four patients receiving long-term opioid therapy in a primary care setting struggles with opioid addiction. Once addicted, it can be hard to stop. In 2016, more than 11.5 million Americans reported misusing prescription opioids in the past year. Taking too many prescription opioids can stop a person's breathing—leading to death.

Prescription opioid overdose deaths also often involve benzodiazepines. Benzodiazepines are central nervous system depressants used to sedate, induce sleep, prevent seizures, and relieve anxiety. Examples include alprazolam (Xanax®), diazepam (Valium®), and lorazepam (Ativan®). Avoid taking benzodiazepines while taking prescription opioids whenever possible.

Side Effects of Prescription Opioids

In addition to the serious risks of addiction, abuse, and overdose, the use of prescription opioids can have a number of side effects, even when taken as directed:

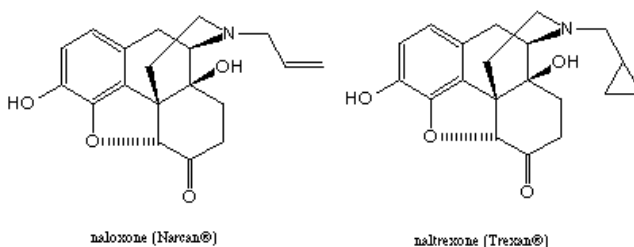
- Tolerance—meaning you might need to take more of the medication for the same pain relief
- Physical dependence—meaning you have symptoms of withdrawal when the medication is stopped
- Increased sensitivity to pain
- Constipation
- Nausea, vomiting, and dry mouth

- Sleepiness and dizziness
- Confusion
- Depression
- Low levels of testosterone that can result in lower sex drive, energy, and strength
- Itching and sweating

Opiate Antagonists

Naloxone, when administered to normal individuals, produces no analgesia, euphoria, or respiratory depression. However, it rapidly precipitates withdrawal in narcotic-dependent individuals. Naloxone antagonizes the actions of morphine at all its receptors.

The uses of naloxone include the reversal of the respiratory depression that follows acute narcotic intoxication and the reversal of narcotic-induced respiratory depression in newborns of mothers who have received narcotics. The use of naloxone is limited by a short duration of action and the necessity of parenteral route of administration.



Naltrexone became clinically available in 1985 as a new narcotic antagonist. Its actions resemble those of naloxone, but naltrexone is well absorbed orally and is long acting, necessitating only a dose of 50 to 100 mg. Therefore, it is useful in narcotic treatment programs where it is desired to maintain an individual on chronic therapy with a narcotic antagonist. In individuals taking naltrexone, subsequent injection of an opiate will produce little or no effect. Naltrexone appears to be particularly effective for the treatment of narcotic dependence in addicts who have more to gain by being drug-free rather than drug dependant.

Combination Pain Relievers

Aspirin is often combined with acetaminophen in a single tablet for relief of arthritis and other painful conditions. Sometimes other drugs such as caffeine, an antihistamine, nasal drying agents, and sedatives are also added. Although some of these preparations may have special uses for certain acute conditions such as a cold or a headache, they should not be taken for a chronic (long-term) form of arthritis. If a combination is required, each drug should be prescribed separately. The dose of each should be adjusted individually to achieve the greatest benefit with the fewest side effects.

Hydrocodone is available in combination with other ingredients, and different combination products are prescribed for different uses. Some hydrocodone combination products are used to relieve moderate-to-severe pain. Other hydrocodone combination products are used to relieve cough. Hydrocodone is in a class of medications called opiate (narcotic) analgesics and in a class of medications called antitussives. Hydrocodone relieves pain by changing the way the brain and nervous system respond to pain. Hydrocodone relieves cough by decreasing activity in the part of the brain that causes coughing.

Web Link

A list of different hydrocodone combination products can be found on the link below.

<https://medlineplus.gov/druginfo/meds/a601006.html>

Summary

- Different types of medicine address different ailments. Anti-inflammatory drugs mediate inflammation, analgesics relieve pain, and antipyretic drugs help lower body temperature associated with fever.
- Over the counter (OTC) pain relievers relieve the minor aches and pains associated with conditions such as headaches, fever, colds, flu, arthritis, toothaches, and menstrual cramps.

- There are basically two types of OTC pain relievers: acetaminophen and non-steroidal anti-inflammatory drugs (NSAIDs).
- Aspirin and other aspirin-like drugs work by blocking the (COX-1 and COX-2) enzymes involved in pain and inflammation.
- Typical prescription pain relief medicines include opioids and non-opioid medications.
- In addition to the serious risks of addiction, abuse, and overdose, the use of prescription opioids can have a number of side effects,

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4.2.1: Pain Relievers- From Aspirin to Oxycodone is shared under a [not declared](#) license and was authored, remixed, and/or curated by LibreTexts.

4.2.2: Cold and Allergy Medicines

Learning Objective

- Know the cause of the common cold and allergies.
- Know the chemical name, common name, and uses of different cough, cold, and allergy medicines.

The **common cold** is a viral infectious disease of the upper respiratory tract which affects primarily the nose. The symptoms of the common cold are believed to be primarily related to the immune response to the virus. Symptoms include coughing, sore throat, runny nose, and fever which usually resolve in seven to ten days, with some symptoms lasting up to three weeks. Well over 200 viruses are implicated in the cause of the common cold. The most commonly implicated virus is a rhinovirus (30–80%).

No cure for the common cold exists, but the symptoms can be treated. Antibiotics have no effect against viral infections and thus have no effect against the viruses that cause the common cold. Due to their side effects they cause overall harm; however, they are still frequently prescribed. It is the most frequent infectious disease in humans with the average adult contracting two to three colds a year and the average child contracting between six and twelve. These infections have been with humanity since antiquity.

Allergies are a number of conditions caused by hypersensitivity of the immune system to typically harmless substances in the environment. These diseases include hay fever, food allergies, atopic dermatitis, allergic asthma, and anaphylaxis. Symptoms may include red eyes, an itchy rash, sneezing, a runny nose, shortness of breath, or swelling. Food intolerances and food poisoning are separate conditions.

Early exposure to potential allergens may be protective. Treatments for allergies include the avoidance of known allergens and the use of medications such as steroids and antihistamines. **Histamine** is concentrated in mast cells, cells whose function is essentially to release histamine and immunoglobins when tissue damage occurs. They are especially numerous in parts of the body that are injured often, such as the fingers and toes, or which enjoy frequent contact with the environment, such as the mucosa of the lips, nose, etc.

Types of Cold and Allergy Medications

Cold medicines are medications used by people with the common cold, cough, or related conditions. While a wide variety of drugs are marketed as cough suppressants, research shows there is often little or no measurable benefit in reducing cough symptoms. While they have been used by 10% of American children in any given week, they are not recommended in Canada or the United States in children six years or younger because of lack of evidence showing effect and concerns of harm. One version with codeine, guaifenesin, and pseudoephedrine was the 213th most commonly prescribed medication in 2017, in the United States, with more than two million prescriptions.

There are a number of different cough and cold medications, which may be used for various coughing symptoms. The commercially available products may include various combinations of any one or more of the following types of substances listed in the table below.

Table 4.2.2.1 Different Cough & Cold Medications.

Medication	Function	Examples
Mucokinetics, or mucolytics	a class of drugs which aid in the clearance of mucus from the airways, lungs, bronchi, and trachea	carbocisteine, ambroxol, and bromhexine.
Expectorants	substances claimed to make coughing easier while enhancing the production of mucus and phlegm.	acetylcysteine and guaifenesin.
Antitussives, or cough suppressants substances which suppress the coughing itself	substances which suppress the coughing itself	codeine, pholcodine, dextromethorphan, noscapine, and butamirate.

Medication	Function	Examples
Antihistamines	for allergic rhinitis may produce mild sedation and reduce other associated symptoms, like a runny nose and watery eyes	diphenhydramine, chlorpheniramine, brompheniramine, loratadine, and cetirizine.
Decongestants	relieve nasal congestion and sinus infection	ephedrine, phenylephrine, pseudoephedrine, and oxymetazoline.
Fever or pain medication (antipyretic or analgesic)	fever reducer or pain reliever	paracetamol (called "acetaminophen " in the US) and NSAIDs such as aspirin, ibuprofen or naproxen
Syrups	various substances supposed to soften the coughing	honey or supplement syrup

Effectiveness

The efficacy of cough medication is questionable, particularly in children. A 2014 Cochrane review concluded that "There is no good evidence for or against the effectiveness of OTC medicines in acute cough". Some cough medicines may be no more effective than placebos for acute coughs in adults, including coughs related to upper respiratory tract infections. The American College of Chest Physicians emphasizes that cough medicines are not designed to treat whooping cough, a cough that is caused by bacteria and can last for months. No over-the-counter cough medicines have been found to be effective in cases of pneumonia. They are not recommended in those who have COPD, chronic bronchitis, or the common cold. There is not enough evidence to make recommendations for those who have a cough and cancer.

Medications

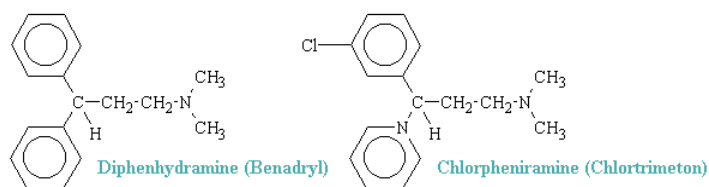
- Dextromethorphan (DXM) may be modestly effective in decreasing cough in adults with viral upper respiratory infections. However, in children it has not been found to be effective.
- Codeine was once viewed as the "gold standard" in cough suppressants, but this position is now questioned. Some recent placebo-controlled trials have found that it may be no better than a placebo for some causes including acute cough in children. It is thus not recommended for children. Additionally, there is no evidence that hydrocodone is useful in children. Similarly, a 2012 Dutch guideline does not recommend its use to treat acute cough.
- A number of other commercially available cough treatments have not been shown to be effective in viral upper respiratory infections. These include for adults: antihistamines, antihistamine-decongestant combinations, benzonatate, anti asthmatic-expectorant-mucolytic combinations, expectorant-bronchodilator combinations, leukotriene inhibitors, ambroxol, and guaifenesin, sometimes with analgesics, antipyretics, anti inflammatories, and anticholinergics - and for children: antihistamines, decongestants for clearing the nose, or combinations of these and leukotriene inhibitors for allergy and asthma. However, antihistamines cannot be used as an empirical therapy in case of chronic, or non specific cough especially in very young children. Long term diphenhydramine use is associated with negative outcomes in older people.

Antihistamines are drugs which treat hay fever and other allergies. Typically, people take antihistamines as an inexpensive, not patented (generic), drug that can be bought without a prescription and relieves from nasal congestion, sneezing, or hives caused by pollen, dust mites, or animal allergy with few side effects. Antihistamines are usually for short-term treatment. Chronic allergies increase the risk of health problems which antihistamines might not treat, including asthma, sinusitis, and lower respiratory tract infection. Consultation of a medical professional is recommended for those who intend to take antihistamines for longer-term use.

Although people typically use the word "antihistamine" to describe drugs for treating allergies, doctors and scientists use the term to describe a class of drug that opposes the activity of histamine receptors in the body. In this sense of the word, antihistamines are subclassified according to the histamine receptor that they act upon. The two largest classes of antihistamines are H₁-antihistamines and H₂-antihistamines.

H₁-antihistamines work by binding to histamine H₁ receptors in mast cells, smooth muscle, and endothelium in the body as well as in the tuberomammillary nucleus in the brain. Antihistamines that target the histamine H₁-receptor are used to treat allergic reactions in the nose (e.g., itching, runny nose, and sneezing). In addition, they may be used to treat insomnia, motion sickness, or vertigo caused by problems with the inner ear. H₂-antihistamines bind to histamine H₂ receptors in the upper gastrointestinal tract,

primarily in the stomach. Antihistamines that target the histamine H₂-receptor are used to treat gastric acid conditions (e.g., peptic ulcers and acid reflux). Two common examples of antihistamines are shown below.



Alternative Medicine

Honey may be a minimally effective cough treatment. A Cochrane review found the evidence to recommend for or against its use in children to be weak. In light of this they found it was better than no treatment, placebo, and diphenhydramine but not better than dextromethorphan for relieving cough symptoms. Honey's use as a cough treatment has been linked on several occasions to infantile botulism and accordingly should not be used in children less than one year old.

Many alternative treatments are used to treat the common cold. A 2007 review states that, "alternative therapies (i.e., Echinacea, vitamin C, and zinc) are not recommended for treating common cold symptoms; however, ... Vitamin C prophylaxis may modestly reduce the duration and severity of the common cold in the general population and may reduce the incidence of the illness in persons exposed to physical and environmental stresses." A 2014 review also found insufficient evidence for Echinacea.

A 2009 review found that the evidence supporting the effectiveness of zinc is mixed with respect to cough, and a 2011 Cochrane review concluded that zinc "administered within 24 hours of onset of symptoms reduces the duration and severity of the common cold in healthy people". A 2003 review concluded: "Clinical trial data support the value of zinc in reducing the duration and severity of symptoms of the common cold when administered within 24 hours of the onset of common cold symptoms." Zinc gel in the nose may lead to long-term or permanent loss of smell. The FDA therefore discourages its use.

Adverse effects

A number of accidental overdoses and well-documented adverse effects suggested caution in children. The FDA in 2015 warned that the use of codeine-containing cough medication in children may cause breathing problems. Cold syrup overdose has been linked to visual and auditory hallucinations, rapid involuntary jaw, tongue and eye movements in children.

Summary

- The **common cold** (also known as nasopharyngitis, rhinopharyngitis, acute coryza, or a cold) is a viral infectious disease of the upper respiratory tract which affects primarily the nose. The symptoms of the common cold are believed to be primarily related to the immune response to the virus.
- An **allergy** is an immune response (with the release of histamines), or reaction, to substances (allergens) that are usually not harmful.
- A number of different cough and cold medications can be used to alleviate various symptoms but not diminish the intensity of the response.

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4.4: Drugs vs. Poisons- All About the Dose

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4.4.1: Natural Poisons and Food Poisoning

Learning Objectives

- List different plant and animal poisons and their properties.
- List various causes of food poisoning.

In biology, **poisons** are substances that cause death, injury or harm to organs, usually by chemical reactions or other activity on the molecular scales, when an organism absorbs a sufficient quantity. The fields of medicine (particularly veterinary) and zoology often distinguish a poison from a toxin, and from a venom. Toxins are poisons produced by organisms in nature, and venoms are toxins injected by a bite or sting (this is exclusive to animals). The difference between venom and other poisons is the delivery method.

The **history of poison** stretches from before 4500 BCE to the present day. Poisons have been used for many purposes across the span of human existence, most commonly as weapons, anti-venoms, and medicines. Poison has allowed much progress in branches, toxicology, and technology, among other sciences.

Over the centuries, the variety of harmful uses of poisons continued to increase. The means for curing these poisons also advanced in parallel. In the modern world, intentional poisoning is less common than the Middle Ages. Rather, the more common concern is the risk of accidental poisoning from everyday substances and products.

Constructive uses for poisons have increased considerably in the modern world. Poisons are now used as pesticides, disinfectants, cleaning solutions, and preservatives. Nonetheless, poison continues to be used as a hunting tool in remote parts of developing countries, including Africa, South America, and Asia.

Poisonous Plants

Poisonous plants are plants that produce toxins that deter herbivores from consuming them. Plants cannot move to escape their predators, so they must have other means of protecting themselves from herbivorous animals. Some plants have physical defenses such as thorns, spines and prickles, but by far the most common type of protection is chemical. Over millennia, through the process of natural selection, plants have evolved the means to produce a vast and complicated array of chemical compounds in order to deter herbivores. Tannin, for example, is a defensive compound that emerged relatively early in the evolutionary history of plants, while more complex molecules such as polyacetylenes are found in younger groups of plants such as the Asterales. Many of the known plant defense compounds primarily defend against consumption by insects, though other animals, including humans, that consume such plants may also experience negative effects, ranging from mild discomfort to death. Several poisonous plants, the specific toxins and the poisonous effects are listed below.

Poison ivy (Figure 4.4.1.1) - The poison Urushiol is an oily mixture of organic compounds with allergic properties. Symptoms of a reaction include itching, redness, swelling, and blisters. It is important to note that the blisters are not contagious.



Figure 4.4.1.1 Poison Ivy.

Western water hemlock (Figure 4.4.1.2) - The toxin, cicutoxin and oenanthotoxin, are conjugated polyacetylenes. These unsaturated alcohols have a strong carrot-like odor and are noncompetitive antagonists for the gamma-aminocutyric acid (GABA) neural transmitter in the central nervous system. GABA role is to inhibit neuron excitability; essentially it has a relaxing function. Blocking this results in convulsing and grand mal seizures and eventually death can occur.



Figure 4.4.1.2 Western water hemlock.

Autumn skullcap - The toxin amatoxin in the form of γ -amanitin, β -amanitin, and α -amanitin causes severe abdominal pain, vomiting, and diarrhea may last for six-nine hours. The toxins affect the liver, results in gastrointestinal bleeding, coma, kidney failure, or even death, within seven days of consumption

Henbane - The toxins in this plant are atropine and scopolamine, found in leaves. Apoatropine and cuscohygrine are the main alkaloids of the root. The main alkaloid in seeds is hyoscyamine, little hyoscyne and little atropine. the plant is toxic to cattle, wild animals, fish, and birds. Pigs are immune. In humans, it could cause hallucinations, dilated pupils, restlessness, fast heart, seizure, vomiting, high blood pressure, and ataxia. Initial effects last for 3-4 hours, after effects last up to three days.

Oak - Tannic acid, binds and precipitates proteins. Cattle, sheep, horses and goats are most affected while pigs are immune. In humans, Tannic acid poisoning could cause anorexia, depression, constipation, diarrhea, blood in urine. Signs typically occur around 3-7 days after consumption, with

The links below are an extensive, if incomplete, list of plants containing one or more poisonous parts that pose a serious risk of illness, injury, or death to humans or domestic animals. There is significant overlap between plants considered poisonous and those with psychotropic properties, some of which are toxic enough to present serious health risks at recreational doses. There is a distinction between plants that are poisonous because they naturally produce dangerous phytochemicals, and those that may become dangerous for other reasons, including but not limited to infection by bacterial, viral, or fungal parasites; the uptake of toxic compounds through contaminated soil or groundwater; and/or the ordinary processes of decay after the plant has died; this list deals exclusively with plants that produce phytochemicals. Many plants, such as peanuts, produce compounds that are only dangerous to people who have developed an allergic reaction to them, and with a few exceptions, those plants are not included here (see list of allergens instead). Despite the wide variety of plants considered poisonous, human fatalities caused by poisonous plants – especially resulting from accidental ingestion – are rare in the developed world.

WEB LINK

A more extensive list of poisonous plants can be found on the link below.

https://en.Wikipedia.org/wiki/List_o...isonous_plants

Poisonous Animals

Several deadly poisons are from snakes and spiders. Several poisonous animals, the specific toxins and the poisonous effects are listed below.

Timber rattlesnake - There are 4 types of toxin. Type A : A neurotoxin known as canebrake. Type B : A hemorrhagic and proteolytic toxin. Type A + B: Intergrade between snakes with Type A and Type B. Type C : relatively weak. The toxins could cause myokymia, defibrination syndrome, numbness, lightheadedness, weakness, vomiting, blurred vision, sweating, salivating. It can be treated with CroFab Antivenom.

Eastern coral snake (Figure 4.4.1.3).- Phospholipase A2 and three-finger toxins (abbreviated as 3FTx). 3FTx proteins are neurotoxins, attacking nerve tissue. Phospholipase A2 can cause inflammation and pain at the site of the bite, though this is

uncommon. The toxins could also cause slurred speech, double vision, muscle paralysis, and can lead to cardiac arrest if left untreated.



Figure 4.4.1.3 *The eastern coral snake*

Cotton mouth snake - Cotton mouth toxins mainly consist of three protein families: phospholipase A2 (PLA2), metalloproteases (SVMP), and serine proteases (SVSP). PLA2s are responsible for inflammation and pain, while SVMPs are responsible for hemorrhage and SVSPs affect the coagulation of blood. The poison could lead to low blood pressure, weakness, change in skin color at site of bite, trouble breathing, nausea, increase in heart rate.

Black widow spider (Figure 4.4.1.4) - Latrotoxins are the main component of the venom, but other compounds such as polypeptides, adenosine, and guanosine are active as well. Only the bite of the female is dangerous to humans, as their venom glands are very large. The toxin can cause pain and sweating at the site of the bite, muscle cramps, headache, nausea, vomiting, weakness. Typically only localized pain is felt, but in some cases the pain can spread. Symptoms typically last from 3-7 days after the bite takes place.

Brown recluse spider - Brown recluse venom possesses potentially deadly hemotoxins and cytotoxins that affect the red blood cells and their ability to clot. It is a mixture of enzymes such as collagenase, protease, and phospholipase. Symptoms include redness, fever, weakness, pain and nausea. In around 10% of victims necrosis can occur at the site of the bite, and in even fewer cases hemolysis (bursting of red blood cells) can occur.



Figure 4.4.1.4 *Western black widow.*

Other Poisonous Animals

The list below is a partial list of animals that are poisonous to humans (and other animals), or put another way, their flesh is toxic if consumed, or in some cases touched:

Birds: Pitohui, Blue-capped ifrit, Little shrikethrush, Spur-winged goose^[1] (diet-dependent), and Common quail (diet-dependent)

Snakes: Rhabdophis keelback snakes and Garter snake (diet-dependent, when feeding on Pacific newts)^[2]

Frogs and toads: American toad, Asiatic toad, Cane toad, Colorado River toad, Common toad, Corroboree frog, European green toad, Fowler's toad, Mantella, and poison dart frog (Figure 4.4.1.5).



Figure 4.4.1.5 Poison dart frogs are well known for their brightly colored skin, which serves as a warning to predators of their toxicity.

Salamanders: Pacific newts

Fish: Tetraodontidae (Blowfish, Pufferfish), Greenland shark, and Barracuda (age and diet dependent)

Cephalopods: Blue-ringed octopus and Pfeffer's flamboyant cuttlefish

Insects: Blister beetle, Birdwings, Milkweed butterfly, Battus (butterfly), Diamphidia, and Monarch (butterfly)

Food Poisoning

Foodborne illness (also **foodborne disease** and colloquially referred to as **food poisoning**)^[1] is any illness resulting from the spoilage of contaminated food, pathogenic bacteria, viruses, or parasites that contaminate food,^[2] as well as toxins such as poisonous mushrooms and various species of beans that have not been boiled for at least 10 minutes.

Many different disease-causing germs (Figure 4.4.1.6 below) can contaminate foods, so there are many different foodborne infections. The US CDC estimates that each year 48 million people get sick from a foodborne illness, 128,000 are hospitalized, and 3,000 die. Researchers have identified more than 250 foodborne diseases. Most of them are infections, caused by a variety of bacteria, viruses, and parasites. Harmful toxins and chemicals also can contaminate foods and cause foodborne illness.

Although anyone can get a foodborne illness, some people are more likely to develop one. Those groups include Pregnant women, Young children, Older adults, People with immune systems weakened from medical conditions, such as diabetes, liver disease, kidney disease, organ transplants, HIV/AIDS, or from receiving chemotherapy or radiation treatment. Most people with a foodborne illness get better without medical treatment, but people with severe symptoms should see their doctor.

Food Poisoning Symptoms

Common symptoms of foodborne diseases are nausea, vomiting, stomach cramps, and diarrhea. However, symptoms may differ among the different types of foodborne diseases. Symptoms can sometimes be severe and some foodborne illnesses can even be life-threatening. Most people have only mild illnesses, lasting a few hours to several days. However, some people need to be hospitalized, and some illnesses result in long-term health problems or even death. Infections transmitted by food can result in chronic arthritis, brain and nerve damage, and hemolytic uremic syndrome (HUS), which causes kidney failure.

Food poisoning symptoms may range from mild to severe and may differ depending on the germ you swallowed (see Table 4.4.1.1 below). After you consume a contaminated food or drink, it may take hours or days before you develop symptoms. See your doctor or healthcare provider if you have symptoms that are severe, including:

- High fever (temperature over 101.5°F, measured orally)
- Blood in stools
- Frequent vomiting that prevents keeping liquids down (which can lead to dehydration)
- Signs of dehydration, including a marked decrease in urination, a very dry mouth and throat, or feeling dizzy when standing up.
- Diarrhea that lasts more than 3 days

The top five germs that cause illnesses from food eaten in the United States are *Norovirus*, *Salmonella*, *Clostridium perfringens*, *Campylobacter*, and *Staphylococcus aureus* (Staph).

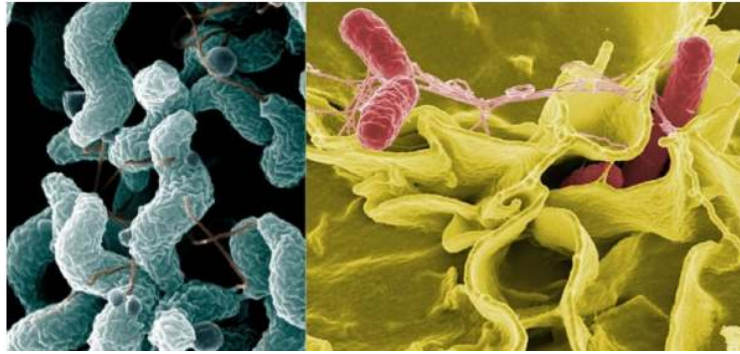


Figure 4.4.1.6 Campylobacter (left) , a bacteria that is a major cause of food poisoning and Salmonella (right). Images used with permission (Public Domain; De Wood, Pooley, USDA (left) and Rocky Mountain Laboratories, NIAID, NIH).

Some other germs don't cause as many illnesses, but when they do, the **illnesses are more likely to lead to hospitalization**. Those germs include *Clostridium botulinum* (botulism), *Listeria*, *Escherichia coli* (*E. coli*), and *Vibrio*.

Table 4.4.1.1 Symptoms and Sources of 10 Foodborne Germs

Germ and Typical Time for Symptoms to Appear	Typical Signs and Symptoms	Common Food Sources
<i>Campylobacter</i> 2 – 5 days	Diarrhea (often bloody), stomach cramps/pain, fever	Raw or undercooked poultry, raw (unpasteurized) milk, and contaminated water
<i>Clostridium botulinum</i> 18 – 36 hours	Double or blurred vision, drooping eyelids, slurred speech. Difficulty swallowing, breathing and dry mouth. Muscle weakness and paralysis. Symptoms start in the head and move down as severity increases	Improperly canned or fermented foods, usually homemade. Prison-made illicit alcohol.
<i>Clostridium perfringens</i> 6 – 24 hours	Diarrhea, stomach cramps. Vomiting and fever are uncommon. Usually begins suddenly and lasts for less than 24 hours	Beef or poultry, especially large roasts; gravies; dried or precooked foods
<i>Cyclospora</i> 1 week	Watery diarrhea, loss of appetite and weight loss. Stomach cramps/pain, bloating, increased gas, nausea, and fatigue.	Raw fruits or vegetables, and herbs
<i>Escherichia coli</i> 3 – 4 days	Severe stomach cramps, diarrhea (often bloody), and vomiting. Around 5-10% of people diagnosed with this infection develop a life-threatening complication.	Raw or undercooked ground beef, raw (unpasteurized) milk and juice, raw vegetables (such as lettuce), and raw sprouts, contaminated water
<i>Listeria</i> 1 – 4 weeks	Pregnant women typically experience fever and other flu-like symptoms, such as fatigue and muscle aches. Infections during pregnancy can lead to serious illness or even death in newborns. Other people (most often older adults): headache, stiff neck, confusion, loss of balance and convulsions in addition to fever and muscle aches.	Raw (unpasteurized) milk, soft cheeses made with raw milk, raw sprouts, melons, hot dogs, pâtés, lunch meats, and cold cuts, smoked seafood

Germ and Typical Time for Symptoms to Appear	Typical Signs and Symptoms	Common Food Sources
Norovirus 12 – 48 hours	Diarrhea, nausea/stomach pain, vomiting	Infected person, contaminated food like leafy greens, fresh fruits, shellfish (such as oysters), or water, or by touching contaminated surfaces
Salmonella 12 – 72 hours	Diarrhea, fever, stomach cramps, vomiting	Eggs, raw or undercooked poultry or meat, unpasteurized milk or juice, cheese, raw fruits and vegetables
Staphylococcus aureus (Staph) 30 minutes – 6 hours	Diarrhea, nausea, stomach cramps, vomiting	Foods that are handled by people and not cooked (sliced meat, puddings, pastries, and sandwiches). Raw (unpasteurized) milk and cheese made from it.
Vibrio 1 – 4 days	Watery diarrhea, nausea, stomach cramps, vomiting, fever, chills	Raw or undercooked shellfish, particularly oysters


The Top 5 Strangest Posions That Can Kill You




Video 4.4.1.1 Strange poisons.

Summary

- Various plants produce toxins that could be lethal or cause allergic reactions in herbivores. A few examples of poisonous plants include poison ivy, western water hemlock, autumn skullcap, henbane, oak, etc.
- Several deadly poisons come from snakes and spiders. Various birds, fishes, frogs, insects, etc. are deadly when consumed or touched due to their toxic flesh.
- The top five germs that cause illnesses from food eaten in the United States are *Norovirus*, *Salmonella*, *Clostridium perfringens*, *Campylobacter*, and *Staphylococcus aureus* (Staph).

Contributors

- Wikipedia
- Scioly.org
- USDA Agricultural Service
- US Center for Disease Control
- Libretexts: Nutrition (Coppola)
- [Marisa Alviar-Agnew](#) (Sacramento City College)

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4.4.2: The Lethal Dose

Learning Objectives

- Describe the LD₅₀ value and its limitations.
- Know the LD₅₀ value of various substances.

The LD₅₀ is a standardized measure for expressing and comparing the toxicity of chemicals. The LD₅₀ is the dose that kills half (50%) of the animals tested (LD = "lethal dose"). The animals are usually rats or mice, although rabbits, guinea pigs, hamsters, and so on are sometimes used. In all these tests, the dose must be calculated relative to the size of the animal. The most common units are milligrams of chemical per kilogram of test animal (mg/kg or ppm). (Table 4.4.2.1) provides examples of LD₅₀ values for various substances.

As a measure of toxicity, lethal dose is somewhat unreliable and results may vary greatly between testing facilities due to factors such as the genetic characteristics of the sample population, animal species tested, environmental factors and mode of administration.

There can be wide variability between species as well; what is relatively safe for rats may very well be extremely toxic for humans (cf. paracetamol toxicity), and vice versa. For example, chocolate, comparatively harmless to humans, is known to be toxic to many animals. When used to test venom from venomous creatures, such as snakes, LD₅₀ results may be misleading due to the physiological differences between mice, rats, and humans. Many venomous snakes are specialized predators of mice, and their venom may be adapted specifically to incapacitate mice; and mongooses may be exceptionally resistant. While most mammals have a very similar physiology, LD₅₀ results may or may not have equal bearing upon every mammal species, including humans.

Table 4.4.2.1: LD₅₀ Values of Various Substances. Source: Wikipedia

Substance	Animal Route	LD ₅₀ (mg/kg)
Water	rat, oral	90,000
Sucrose (table sugar)	rat, oral	29,700
Glucose (blood sugar)	rat, oral	25,800
Monosodium glutamate (MSG)	rat, oral	16,600
Cadmium sulfide	rat, oral	7,080
Ethanol (grain alcohol)	rat, oral	7,060
Methanol	human, oral	810
Sodium chloride (table salt)	rat, oral	3,000
Metallic arsenic	rat, oral	763
Arsenic trisulfide	rat, oral	185-6400
Sodium cyanide	rat, oral	6.4
Hydrogen cyanide	mouse, oral	3.7
Ibuprofen	rat, oral	636
Aspirin	rat, oral	200
Caffeine	rat, oral	192
Cocaine	mouse, oral	96
Nicotine	rat, oral	50
Heroin (diamorphine)	mouse, intravenous	21.8
Methamphetamine	rat, intraperitoneal	57

Substance	Animal Route	LD ₅₀ (mg/kg)
Mercury(II) chloride	rat, oral	1
Strychnine	human, oral	1-2
Sarin	mouse, subcutaneous injection	172 microgram/kg
Ricin (from castor oil plant)	rat, oral	20-30
Botulinum toxin (Botox)	human, oral injection, inhalation	1 ng/kg

(Table 4.4.2.2) gives the LD₅₀ values of some insecticides. In each case, the chemical was fed to laboratory rats. Note that the lower the LD₅₀, the more toxic the chemical. Even adjusting for the test animal's weight, the LD₅₀ for one species is often quite different from that for another. Thus any LD₅₀ value gives only a rough estimate of the risk to humans. The way in which the chemical is administered also has a marked effect on LD₅₀ values. The chemical may be fed, injected, applied to the animal's skin, etc., and each method usually generates a different LD₅₀.

Table 4.4.2.2: LD₅₀ Values of Pesticides.

Chemical	Category	Oral LD ₅₀ in Rats (mg/kg)
Aldicarb ("Temik")	Carbamate	1
Carbaryl ("Sevin")	Carbamate	307
DDT	Chlorinated hydrocarbon	87
Dieldrin	Chlorinated hydrocarbon	40
Diflubenzuron ("Dimilin")	Chitin inhibitor	10,000
Malathion	Organophosphate	885
Methoprene	JH mimic	34,600
Methoxychlor	Chlorinated hydrocarbon	5,000
Parathion	Organophosphate	3
Piperonyl butoxide	Synergist	7,500
Pyrethrin	Plant extract	200
Rotenone	Plant extract	60

Summary

- The LD₅₀ is the dose that kills half (50%) of the animals tested (LD = "lethal dose"). It is a standardized measure for expressing and comparing the toxicity of chemicals.
- LD₅₀ values are given for common drugs (e.g. ibuprofen and aspirin), common household ingredients including water, table sugar (sucrose), salt (sodium chloride), insecticides (e.g. DDT and pyrethrin), and harmful drugs (e.g. cocaine and heroin).

Contributors and Attributions

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