Molecules and Other Matters

3

3.1 The Atom

Most brewers in the pre-1900 world had never heard nor thought about the atom. But the atom was actually postulated to exist long before its discovery. Scientists in Europe developed a series of basic laws and theories about our world in the 1700s and 1800s that did include statements about the atom. For example, John Dalton in 1805 proposed what he called the atomic theory. The statements in this theory largely proved to be correct even after the atom was discovered.

The atom is the smallest unit of everything. Your desk, the pencil, and even the paper upon which you write are composed of atoms. In fact, the atom is so important to science that the periodic table (see Fig. 3.1) occupies a predominant place in nearly every science practiced on this planet. The periodic table lists each of the known elements, some are only known because they are made in the laboratory, and the others are naturally occurring and found in the world around us.

The periodic table is broken down into two main regions denoted by the stair-step line on the right-hand side of the table. To the left of this line are all of the elements that we call metals. Metals are shiny, malleable, ductile, and can conduct both heat and electricity. To the right of the line are all of the elements that we call nonmetals. Nonmetals are just the opposite of metals in that they are dull, brittle, unable to be stretched, and insulate against heat and electricity. Elements that touch the line are known as the metalloids because they have properties that are half way between those of the metals and the nonmetals.

The elements in the Periodic table are arranged based upon their physical characteristics and properties, such as their reactivity with water. For example, the elements in the first group or column in the table react quickly with water to make alkaline solutions. The arrangement also accounts for the sizes of the elements; the atoms get small as you move across a row, and larger as you move down a column.

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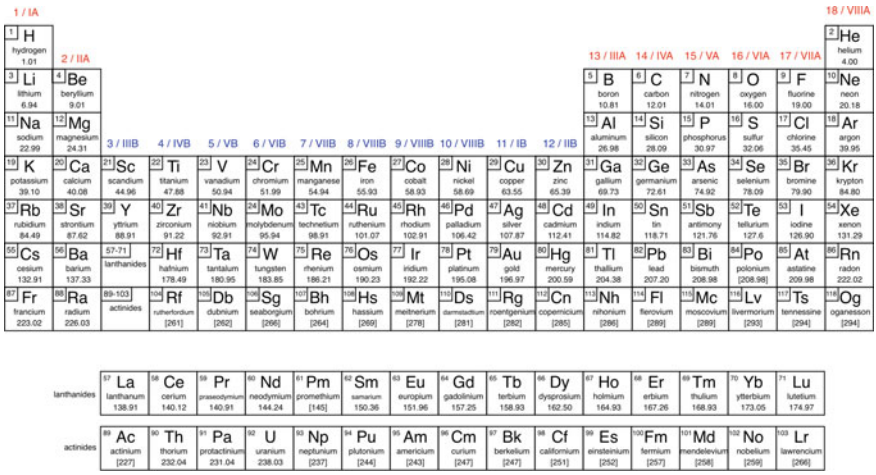


Fig. 3.1 The periodic table

Because of the way in which the atoms were placed into the periodic table, each column (or Group) contains atoms that have fairly similar properties. And most of the Groups have names that describe the key features. For example, the last Group is known as the noble gases because the atoms that make up that group are fairly unreactive gases. Group 1 are the alkali metals because of their reactivity, Group 2 are the alkaline earth metals (they react with water to make alkaline solutions, too), Group 11 is known as the coinage metals (copper, silver, gold), and Group 17 are the halogens.

The atom can be thought of as a very tiny solar system. At its center where the Sun would be is a collection of smaller particles known as protons and neutrons. This collection of particles is known as the nucleus of the atom. Protons and neutrons have essentially the same mass; the mass of each is approximately equal to 1 atomic mass unit (amu). Because the protons have a positive charge and the neutrons have no charge, the nucleus overall has a positive charge. Of these two particles, the proton is the most important because the number of protons dictates the specific element on the periodic table. The number of protons in an atom, in other words, determines the type of atom. That number is the whole number written in each box in the periodic table. For example, carbon has six protons and oxygen has eight.

The number of neutrons in a nucleus can vary and, in most cases, is not equal to the number of protons in the nucleus. When an element has more than one option, the result is an isotope. Some isotopes even have different names. For example, hydrogen can be found in three different forms in nature. One form has no neutrons in the nucleus (known as hydrogen), one has only one neutron (known as deuterium), and the other has two neutrons (known as tritium). While isotopes seem to compound our understanding of the periodic table, the good news is that even with multiple isotopes, to the first approximation, the properties of each are still the same

as the other. In other words, if the nucleus has 1 proton, the atom is hydrogen regardless of the number of neutrons it possesses.

Surrounding the nucleus of the atom is a sea of particles called electrons. These very fast moving particles have a negative charge. But because electrons have a mass that is 1/1000th the size of the mass of a proton or a neutron, the overall mass of the atom is essentially equal to the mass of all of the protons and neutrons. In other words, electrons can be thought of as having almost no mass. In addition, in order to have an atom without a net charge, the number of electrons (the negatively charged particles) must equal the number of protons (the positively charged particles). Thus, the carbon atom must have six electrons circling the nucleus; there must be eight electrons around the oxygen nucleus.

CHECKPOINT 3.1

How many protons, neutrons, and electrons are in an atom of nitrogen that has a total mass of 14 amu? …in an isotope of nitrogen with a mass of 16 amu?

What element would contain 11 protons, 12 neutrons, and 11 electrons?

Unfortunately, it is rare to find one of the elements of the periodic table with the correct number of electrons around the atom. This is because electrons are used to bind atoms together. When the number of electrons is different than the number of protons, the atom becomes an ion. A positively charged ion, called a cation (pronounced CAT-ION), has fewer electrons than protons. The negatively charged ion, called an anion (pronounced AN-ION), has more electrons than protons. Knowing that protons have a +1 charge and electrons have a −1 charge, it makes sense that a cation would have fewer electrons than protons.

What would be the charge on an ion of carbon if it had only four electrons? We could answer this question by noting that there are always six protons in a carbon atom, and with only four electrons, there would be two protons that were not balanced by electrons. The charge would be 2+. Similarly, an oxygen ion with 10 electrons would have a 2− charge.

As it turns out, when atoms bond with other atoms they tend to gain or lose electrons based on their location in the periodic table. Metal atoms tend to lose the same number of electrons as the atoms position along the period. This is particularly true for metals in Group 1 and Group 2. The result is a cation with a charge that is equal to the Group number, e.g., H^+, Li^+, Mg^{2+}, and Ca^{2+}. Aluminum is the third element in the period, so it would have a charge of 3+; Al^{3+}. The "transition metals" in Group 3 through Group 12, however, tend to have multiple possibilities, although a 2+ charge is very common; e.g., Ti^{2+}, Ni^{2+}, Fe^{2+}, Fe^{3+}.

Nonmetals tend to form anions with the charge equal to the number of elements remaining in the period. Nitrogen is three "boxes" away from the end of the row, so it would be N^{3-}; oxygen is two boxes from the end of the row, so it would be O^{2-}.

While this rule tends to work often, most of the nonmetals have multiple possibilities for their anion charges. The halogens almost always have a 1− charge.

CHECKPOINT 3.2
What is the charge on a sodium ion with only 10 electrons?
What is the charge on a chlorine ion with 18 electrons?

3.1.1 Compounds

Compounds are formed when two or more atoms combine. For example, water (H_2O) is a compound made from two hydrogen atoms and one oxygen atom. Salt, also known as sodium chloride (NaCl), is a compound made from one atom of sodium and one atom of chlorine. While these two compounds appear to be very similar when we write them, they are very different when we explore how the elements are combined.

The combination of a metal and a nonmetal gives rise to an *ionic compound*. For example, NaCl is an ionic compound. In fact, the metal in an ionic compound (the Na in NaCl) actually exists as a cation; it has fewer electrons than protons. The nonmetal in an ionic compound (the Cl in NaCl) is actually an anion containing more electrons than protons. The positive charge of the cation interacts very strongly with the negative charge of the anion, and an ionic compound results. This electrostatic attraction is very strong force and can be thought of like the attraction between the north pole and south pole of two magnets.

When the ions combine, they do so such that the total charge of the cation(s) is equal to the total charge of the anion(s). For example, in sodium chloride, the sodium ion has a 1+ charge and the chloride ion has a 1− charge. Therefore, one sodium cation must combine with one chloride anion so that the overall charge for the ionic compound is zero. In another example, when calcium cations combine with chloride anions, they do so such that one calcium cation (Ca^{2+}) pairs with two chloride anions (Cl^-) to make $CaCl_2$.

While the force of attraction between oppositely charged ions is very large, some ionic compounds can dissolve and dissociate into their separate ions in water. Sodium chloride, when added to water, dissolves into the water and becomes Na^+ and Cl^-. Calcium chloride also does this, resulting in a water solution of Ca^{2+} and Cl^- ions, though in this case there are twice as much Cl^- anions in solution as Ca^{2+} cations. But not all ionic compounds dissolve in water. As we will see later, apatite (an ionic compound) does not dissolve in water, nor does it dissociate into its ions.

Compounds can also contain nothing but elements from the nonmetal side of the periodic table. These combinations are called *molecules*. Carbon monoxide (CO) and water (H_2O) are examples of molecules. In molecules, the atoms do not exist as ions. Instead, the atoms share their electrons so that the electrons encircle all

of the nuclei in the molecule. The forces holding the atoms together are a little weaker than in the ionic compounds, but strong enough to keep the molecules together so that they do not dissociate into ions in water. The atoms in a molecule are said to be joined by covalent bonds.

Just like the ionic compounds, some molecules can dissolve freely in water and some cannot. For our purposes, those containing nitrogen, oxygen, sulfur, or phosphorus tend to be fairly water soluble. Those that lack these atoms or have significantly more carbon atoms than nitrogen, oxygen, sulfur, or phosphorus, tend to not dissolve very well in water. With just a couple of exceptions that we will discuss later, molecules do not dissociate into ions when added to water.

Naming Ionic Compounds Rules for constructing the names of compounds, known as chemical nomenclature, have been set by the International Union of Pure and Applied Chemistry (IUPAC). Those rules define the steps used to determine the name of almost any compound in the world. Ionic compounds are named by saying the name of the cation, and then saying the name of the anion. The ending of the anion is changed so that the entire name ends in "ide." There are modifications to this rule; oxygen as an anion is known as "oxide." Other examples include salt (NaCl), known as sodium chloride, and $BeCl_2$, known as beryllium chloride.

Note that even if the ionic compound contains multiples of either of the ions, we do not state so in the name. For example, calcium bromide has the formula $CaBr_2$. Table 3.1 lists some common ionic compounds and their names.

Polyatomic ions Unfortunately, it is possible that one of the ions in an ionic compound is made up of a molecule (see below) that does not have the correct number of electrons to balance all of its protons. In these cases, a polyatomic ion is born. The polyatomic ion could be a cation, such as NH_4^+, or an anion, such as PO_4^{3-}. When encountered in an ionic compound, the polyatomic ion is not treated any differently than a cation or anion, except that it has a special name that must be used. Table 3.2 lists the names of the common polyatomic ions found in ionic compounds common in the brewery.

Table 3.1 Common binary ionic compounds

Formula	Name	Formula	Name
NaCl	Sodium chloride	KCl	Potassium chloride
$CaCl_2$	Calcium chloride	$MgCl_2$	Magnesium chloride
CaO	Calcium oxide	MgF_2	Magnesium fluoride

Table 3.2 Common polyatomic ions

Formula	Name	Formula	Name
OH^-	Hydroxide	HCO_3^-	Bicarbonate
CO_3^{2-}	Carbonate	PO_4^{3-}	Phosphate
SO_4^{2-}	Sulfate	SO_3^{2-}	Sulfite
NO_2^-	Nitrite	NO_3^-	Nitrate
CH_3COO^-	Acetate	NH_4^+	Ammonium

For example, $Ca(OH)_2$ is commonly known as slaked lime. Its chemical name is calcium hydroxide. NH_4Cl is ammonium chloride. $MgSO_4$, found in Epsom salts, is known as magnesium sulfate. And $Ca_3(PO_4)_2$ is known as calcium phosphate. Note in the formula for calcium phosphate, there are three Ca^{2+} cations and two PO_4^{3-} anions. The total positive charge is 6+ and the total negative charge is 6− in order to balance. Parentheses are used in the formula so that we know if more than one of the polyatomic ions is used in the compound. Also note that when a compound contains these polyatomic ions, they are treated no different than if they were a single entity. This is because they are a single ion, and the parentheses are there to indicate how many of these polyatomic ions are in the formula.

Multiple Charges While it seems like a further complication, chemical naming rules also provide ways to determine the name of a compound where the metal may exist as more than one cation. Remember, the transition elements likely are cations with a 2+ charge, but other charges are very possible. In those cases, the same metal may have multiple formulas with the same atoms, such as in FeO and Fe_2O_3. This is very common.

To name compounds containing a transition element, the charge is placed in the name as a Roman numeral in parentheses. For example, $CuCl_2$ is named copper(II) chloride and CuCl is named copper(I) chloride. Note that no space is placed between the parentheses and the name of the metal. These are actually different compounds with very different properties, and the name must contain the Roman number, so they can be distinguished from each other.

Sometimes, we are presented with an ionic compound containing a transition metal that has a charge that we do not know. By examining the other atoms in the formula, however, it is often easy to determine the charge on the transition metal. For example, it has been shown that 2+ cations can increase the bitterness in beer by reacting with the hop acids. Would $NiCl_2$ suffice to perform this task? Since the nickel is a transition metal, we cannot immediately determine the charge by considering its location on the Periodic table. However, since the halogens almost always have a −1 charge, we can determine the charge on the anion Cl is 1−. With two of these in the formula, the total anionic charge would be 2−. Thus, the nickel must have a charge of 2+ to balance the 2−. The name of the compound would be nickel(II) chloride, and we would predict that it should be able to increase the bitterness in beer by reacting with the hop acids.

Table 3.3 Ionic compounds that use Roman numbers

Formula	Name	Formula	Name
$FeCl_2$	Iron(II) chloride	Fe_2O_3	Iron(III) oxide
$FeCl_3$	Iron(III) chloride	FeO	Iron(II) oxide
AgCl	Silver(I) chloride	TiO_2	Titanium(IV) oxide
$Cu(NO_3)_2$	Copper(II) nitrate	$Mn_3(PO_4)_2$	Manganese(II) phosphate
$CuNO_3$	Copper(I) nitrate	$CuSO_4$	Copper(II) sulfate

Table 3.3 lists some common ionic compounds that require the use of the Roman numeral when writing their names. Many of these compounds are potentially found in brewery waters, are found as contaminants in ingredients, or get accidentally added to the process stream due to the contact of the wort and beer with metals in the brewery. Note that all of these contain transition elements that have multiple cationic charges possible.

Naming Molecules The names of ionic compounds result because of the limitations of compounds that can be made from specific cations and anions. For example, there is only one combination of calcium cations, Ca^{2+}, and chloride anions, Cl^-. The result is calcium chloride ($CaCl_2$). There are only two combinations of copper cations and chloride anions that are common (CuCl and $CuCl_2$).

This restriction does not occur in molecules that result from the combination of nonmetals with nonmetals. Molecules differ not only in the types of bonds that hold the atoms together, but also because the individual atoms in the molecule are not cations and anions, they can be put together in almost every possible combination. For example, the combination of carbon and hydrogen can result in molecules with formula such as CH_4, C_2H_4, C_2H_6, C_3H_8, and thousands and thousands of other formula. Thus, molecules by necessity must be named differently than ionic compounds.

For molecules that only contain two types of atoms, the process of naming is very similar to how the ionic compounds are named. These compounds, known as binary molecules, are named by adding prefixes to the names of the atoms in the formula and changing the ending of the last atom to "–ide." The prefixes we use for this are:

1. Mono	6. Hexa
2. Di	7. Hepta
3. Tri	8. Octa
4. Tetra	9. Nona
5. Penta	10. Deca

There are a couple of modifications we make to the name of the molecule so that it is easier to say. First, we tend to only use the first syllable of the name for the

Table 3.4 Common binary molecules

Formula	Name	Formula	Name
CO	Carbon monoxide	CO_2	Carbon dioxide
NO	Nitrogen monoxide	NO_2	Nitrogen dioxide
SO_2	Sulfur dioxide	N_2O_2	Dinitrogen dioxide
CS_2	Carbon disulfide	P_2S_4	Diphosphorus tetrasulfide
N_2O	Dinitrogen monoxide	N_2O_4	Dinitrogen tetroxide

second atom and then add "–ide." Thus, oxygen as the second atom in the formula becomes "oxide," sulfur becomes "sulfide," phosphorus becomes "phosphide," etc. Second, if the second atom is oxygen, we drop the "a" from the prefix if it has one. And third, if there is only one of the first atoms in the formula, we do not add the "mono" prefix. As examples, CO becomes carbon monoxide, CS_2 becomes carbon disulfide, P_2O_5 is known as diphosphorus pentoxide, ClO_2 is known as chlorine dioxide, and N_2O_3 is named dinitrogen trioxide. Table 3.4 lists some common binary molecules and their names.

Binary molecules that contain both carbon and hydrogen are not named this way. This type of compound because of the multiple ways that the atoms can be arranged requires a special set of naming rules. As we will see later in this chapter, their names are based upon the specific arrangements of the atoms. The special rules emphasize the fact that with a larger number of atoms, many different ways to arrange the atoms become possible. Where with ionic compounds and binary molecules only one way to arrange the atoms is possible, only one name is needed to describe that arrangement. But with multiple ways to arrange the atoms, it is likely that each arrangement is a different compound with different properties. So, each arrangement needs a separate name. For example, there are two different compounds with the formula C_4H_{10} resulting from different arrangements of the atoms (butane and isobutane). The name of the molecule in these cases must be able to distinguish each of these molecules.

3.2 Laws that Govern Atoms, Molecules, and Ionic Compounds

Scientists began asking questions about the world many centuries ago. They mixed different compounds together and observed what happened. They discovered new compounds and new elements and explored their properties. In their search for explanations of the world, they discovered the underlying rules for how and why chemicals exist and react.

A Greek philosopher, Democritus (460–370 BC), came up with one of the earliest theories that helped shape the field of chemistry. Without experimentation, he reasoned that matter (the stuff around us) must be made up of small indivisible

particles. For example, if you have a cup of sand and remove half of it, you would have a half a cup of sand. If you continued to divide it into halves, eventually you would get down to the point where you would have only one sand particle that could not be divided in half. Chemists later realized that this was correct. All matter is made up of particles (atoms), the smallest thing possible. This gave rise to our current understanding of the atom.

As scientists started experimenting with the world around them, they discovered that not all atoms were the same (in fact, we now know of 118 different elements that make up the Periodic table). How those atoms combined to make different compounds became the focus of the majority of their research. The result was a series of laws that govern the modern practice of chemistry.

The first of these chemical laws makes sense in today's world, but at the time the law was being formulated, it was met with great skepticism. The law of constant composition came to be understood by Joseph Proust (French chemist, 1754–1826). The essence of the law is that the formula for a compound is the same, no matter what the source of the compound. For example, water's formula is H_2O, whether it is water from a mountain spring or water obtained from a well. The formula for water is also the same whether it is obtained from natural sources or made in the laboratory. Thus, "natural" vitamin C is exactly the same compound as "synthetic" vitamin C that is made in the laboratory. The formula for both is the same, the structures for both are the same, and the properties are the same.

About the same time that chemists understood how formula were constructed, John Dalton (English chemist, 1766–1844) proposed the law of multiple proportions. The law states that atoms mix in whole number ratios as they form compounds. For the brewer, this means that a formula must contain whole numbers of atoms. For example, mixing oxygen atoms with a carbon atom allows the formation of CO or CO_2, but not $CO_{1.5}$. Again, this law seems logical to us in today's world, but at the time of its discovery this was groundbreaking information.

John Dalton expanded upon his understanding of formula and presented his Atomic Theory around 1806. This theory declared that (a) all matter is made up of atoms, (b) atoms are indivisible and indestructible, (c) compounds are formed by the combination of two or more atoms, and (d) chemical reactions are simply the rearrangement of atoms to form new compounds. While some slight modifications to this theory have been made since the 1800s due to our better understanding of chemistry, most of what he originally postulated in his theory is still correct today.

Let us go back to our understanding of water and look at the chemical equation below. It describes the reaction of hydrogen gas and oxygen gas to make gaseous water. Each of the compounds involved in the chemical reaction is represented by a separate formula made up of atoms. The equation also illustrates that the reaction occurs by simply rearranging atoms from the compounds of hydrogen and oxygen to make the product of the reaction, water. No new atoms are created, and none are destroyed in the reaction (there are the same number of atoms on the left side of the arrow as there are on the right side of the arrow).

$$2H_2(g) + O_2(g) \rightarrow 2H_2O(l) \tag{3.1}$$

The equation also illustrates how we write chemical reactions. On the left side of the equation are the compounds that react together, known as the reactants. On the right side of the equation are the compounds that result from the reaction, known as the products. An arrow that can be read as "reacts to make" or "yields" separates the left and right side of the equation. The letter in parentheses after each chemical formula indicates the state of the compound. In this reaction, the hydrogen and oxygen are gases denoted with an italics "*g*". The water is denoted with an italics "*l*", indicating the water is liquid. Solid compounds are designated with an italics "*s*". The equation is also balanced. This means that it has the same number of each type of atom on both sides of the equation. For example, there are four hydrogen atoms on the left side (the reactants) and four hydrogen atoms on the right side (the products). The large number in front of each compound is used to help make sure the equation is balanced.

Overall, then, the equation can be read as "2 molecules of hydrogen gas and 1 molecule of oxygen gas react to make 2 molecules of liquid water." Note that the "1" is implied even though it is not specifically written in the equation.

Let us look at another example to further illustrate the use of equations. For example, when a solution of calcium bicarbonate is heated, it reacts to make solid calcium carbonate, carbon dioxide, and water (Eq. 3.2). This reaction is very important to the brewer that uses calcium-rich waters in their brewing process. It indicates that by heating the water, the amount of calcium dissolved in the water can be reduced (while also reducing some of the alkalinity of the water).

$$Ca(HCO_3)_2\,(aq) \rightarrow CaCO_3\,(s) + CO_2\,(g) + H_2O\,(l) \tag{3.2}$$

A quick look at the number of atoms on each side of the arrow tells us that the reaction is balanced without adding any numbers in front of the compounds. However, we do notice the italics "*aq.*" This means that the compound is dissolved in water as an "aqueous solution." The equation can be read as "1 formula unit of aqueous calcium bicarbonate yields 1 formula unit of solid calcium carbonate, 1 molecule of gaseous carbon dioxide, and 1 molecule of liquid water." Note that because calcium bicarbonate and calcium carbonate are ionic compounds, they are referred to as formula units instead of as molecules.

Antoine Lavoisier (French chemist, 1743–1794) studied reactions like this. He noted that the weight of the compounds before the reaction began was the same as the total weight of all of the products after the reaction was complete. He noted that no weight was lost in any of the reactions that he performed. Today, we call this the law of the conservation of mass. This law states that chemicals are neither created nor destroyed in a reaction; chemicals may change their identity, but the overall mass does not change. In the brewery, this means that if we add 10 lb of crystal malt to the mash, we will get 10 lb of extracted sugars and leftover grist (after drying it). While the law does not dictate how much of each product we will get, we

know that the total mass of the products is the same as what we started with and nothing just disappears in the reaction. This law works for every chemical reaction.

In the late 1800s, scientists noted some interesting outcomes of their study of chemical formula. They realized that the formulas for some chemical compounds were the same as others. For example, the formula for glucose and fructose are the same ($C_6H_{12}O_6$), even though the compounds were very different. This implied that while the formula for the two compounds was the same, the arrangements of the atoms in the molecules must be different. Glucose and fructose are examples of constitutional isomers. Their formulae are the same, but their constitution (how the atoms are arranged) is different. Thus, the arrangement of atoms in a chemical compound is very important to knowing the identity of the compound. And to carry that even further, the arrangement of atoms is important to understanding the properties of the compound.

How the atoms were arranged around each other in molecules was determined in the late 1800s. In some cases, it was determined that atoms were attached to other atoms by a single bond, such as the bonds that make up the molecule of water (H–O–H). In other cases, it was found that multiple bonds held the atoms together (Fig. 3.2). How these arrangements are constructed will be covered in the next section of this chapter.

In some cases, it was discovered that some compounds with the same formula and the same attachment of atoms still differed in the properties that they expressed. This difference was primarily found in how the compounds interacted in biological systems. For example, the active ingredient in caraway seeds and the active ingredient in spearmint are molecules with the same formula and same attachments of atoms (see Fig. 3.3). But, the taste of these two compounds is very different; one tastes like caraway and the other like spearmint. The difference in the two compounds results from the three-dimensional arrangement of the atoms. This is known as stereoisomerism. While the names of the two compounds are the same, the difference is noted by the addition of a single letter just before the name. The importance of this will be covered in greater detail in the next section.

Another example of stereoisomerism is even more striking. Glucose and galactose have the same formula and structure, but as stereoisomers, they are very different sugars. Both are sweet to the taste, but galactose is much less sweet than glucose. Glucose is found almost everywhere (it is the sugar that makes up starch and cellulose); galactose is part of the sugar that makes up lactose found in milk. In

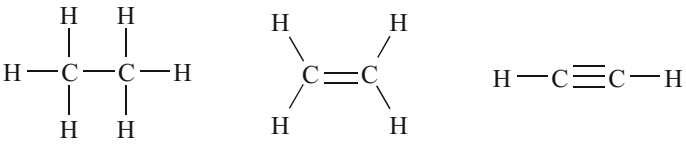


Fig. 3.2 Examples of molecules with multiple bonds. The number of bonds between the two carbon atoms in each structure is represented with multiple lines

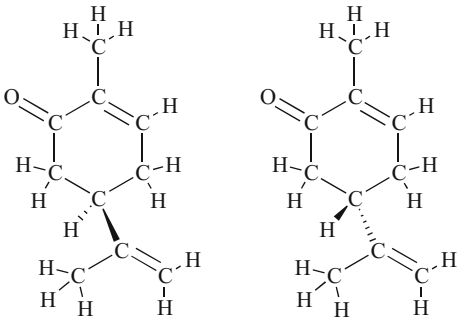


Fig. 3.3 *R*-carvone and *S*-carvone are stereoisomers. They differ only in the three-dimensional arrangement of atoms in the structure of the molecules

another example, D-glucose and L-glucose have the same formula and structure, but are stereoisomers of each other. Both are similar in sweetness, but L-glucose cannot be metabolized by the body and cannot be used to make energy in the body.

CHECKPOINT 3.3
Write the formula for nitrogen disulfide, magnesium carbonate, and cobalt (II) phosphate.
Write the chemical reaction that is described by "one formula unit of solid calcium carbonate reacts to make one formula unit of solid calcium oxide and one gaseous molecule of carbon dioxide."
Based on the law of conservation of mass, explain the "reaction" that occurs when noodles are cooked in boiling water.

3.3 The World of Carbon-Containing Molecules

There are millions of molecules that are known to exist in this world. And millions more are yet to be discovered. While many of these molecules do not contain the element carbon, a significant majority of them do. And many of those that do contain carbon are very important to life. In fact, an entire field of chemistry, known as organic chemistry, focuses on these molecules. Because many of the compounds found in beer contain carbon, the efforts of scientists that study organic chemistry have given the brewer, and the rest of the world, a much clearer picture of what is occurring during the brewing process.

Organic molecules containing carbon are often divided into different classes based upon the arrangement of the atoms in the compound. These classes allow the average scientist to estimate the properties of the millions of compounds without

requiring personal experience with each molecule. Those arrangements that are most important to the brewer only contain the atoms carbon, hydrogen, oxygen, nitrogen, and/or sulfur. Thus, by studying those classes that contain these atoms, the brewer can get a very good sense of the reactions and properties that are possible. The arrangements of these atoms in an organic molecule are known as functional groups.

3.3.1 Basic Functional Groups in Brewing

Hydrocarbon The simplest molecules that contain carbon and hydrogen atoms are known as the hydrocarbons. These molecules contain only atoms of carbon and hydrogen, as the name implies. They are commonly found in nature as petroleum resources such as natural gas and oil, and in natural plant materials, such as waxes and oils.

The simplest of the hydrocarbons is methane (CH_4). Methane is one of the main components that make up natural gas. Methane is very useful as a fuel, and when it reacts with oxygen (combustion), the atoms rearrange to make carbon dioxide and water. The other product of this reaction is heat. It is the heat that is so important and the thing that makes methane so useful. The heat of the reaction with oxygen can be used to generate electricity, warm our houses, or heat our water. Note that based on the formula for methane, the carbon must be attached to four hydrogen atoms. This is a characteristic of carbon—it prefers to make four attachments or bonds to other atoms. This characteristic makes drawing the structure of organic molecules fairly easy. We will cover this in more detail as we proceed through our exploration of functional groups.

Other hydrocarbons include ethane (C_2H_6), propane (C_3H_8), and butane (C_4H_{10}). Propane and butane are used a lot in the USA as fuels. Propane is the gas used in bar-b-que grills and butane is the gas used in cigarette lighters. Each of the hydrocarbons has fairly similar properties. They have fairly low boiling points and low melting points. In addition, as a class of compounds, the hydrocarbons tend not to be soluble in water in large quantities; however, very tiny amounts do dissolve. Some examples and their structures are shown in Fig. 3.4.

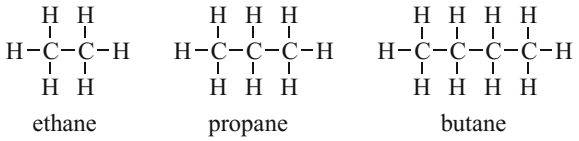


Fig. 3.4 The structure of some hydrocarbons, ethane, propane, and butane. Note that every carbon atom has 4 bonds and every hydrogen atom has 1 bond

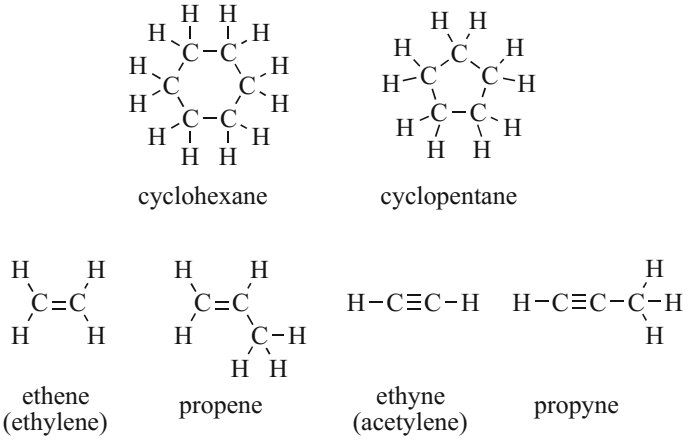


Fig. 3.5 Examples of hydrocarbons that are missing pairs of hydrogen atoms. Note that the carbon atom still has four bonds and the hydrogen atom requires one bond

In some cases, the hydrocarbon is missing a pair of hydrogen atoms. This results in two options for the structure of the compound. It could be represented by a ring of carbon atoms, or it could be represented with a double bond between somewhere in the molecule. Compounds containing a ring of carbon atoms are very common in nature; the six-membered ring occurs in many compounds (see Figs. 3.3 and 3.5). If the molecule has a double bond, it represents a new class of compound known as the alkene. Examples include ethylene and propene (Fig. 3.5). In other cases, the hydrocarbon is missing multiple pairs of hydrogen atoms. This gives rise to the alkyne class of compound. Examples include ethyne and propyne (Fig. 3.5). Both alkenes and alkynes are able to react with other chemicals to make new compounds.

Branching While a long chain of carbon atoms can be drawn for a formula, many of the different ways to draw an organic molecule are the result of branching. This branching is the reason that a single formula results in multiple constitutional isomers. For example, the formula C_6H_{14} can give rise a multitude of structures that represent branched compounds. Figure 3.6 lists the possible hydrocarbons with this formula. Note that each has a different name: The longest carbon chain forms the parent portion of the name. More on the naming of organic compounds is presented in Sect. 3.4.

Ether If an oxygen atom is introduced into the hydrocarbon formula, there become quite a few different possible functional groups. In one arrangement, the oxygen atom is attached to two carbon atoms. This arrangement gives rise to a class of compound we know as the ether functional group. The structure of an ether, coupled with other information we know about oxygen from the formula of water, indicates that oxygen prefers to have two bonds in compounds that it makes.

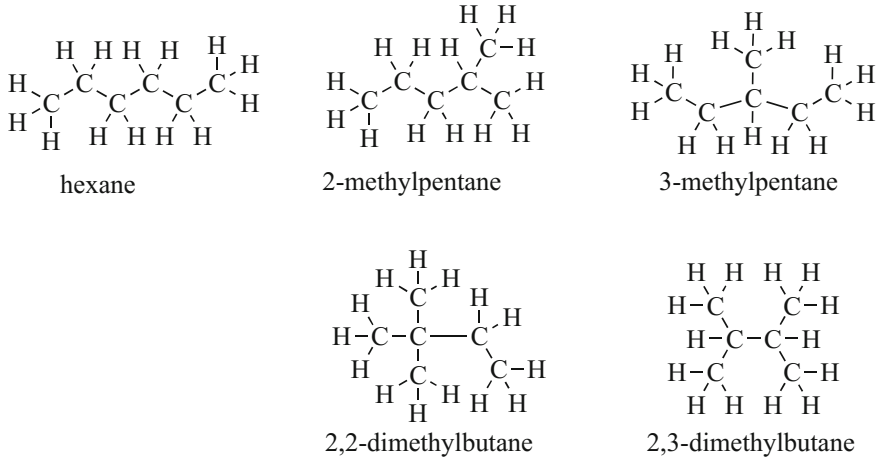


Fig. 3.6 The constitutional isomers of C_6H_{14}. Note that the longest carbon chain is the parent name (6 = hexane, 5 = pentane, and 4 = butane) and that the branches are numbered along that chain

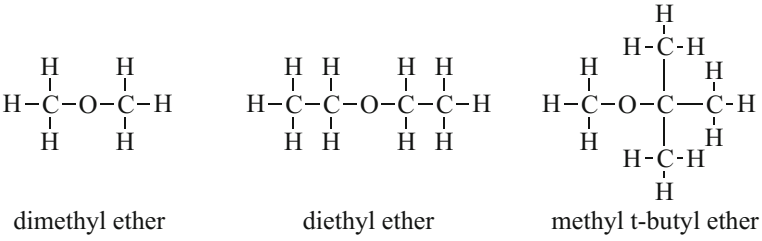


Fig. 3.7 The structure of some ethers. Note that the oxygen atom forms two bonds with other atoms in the structures it forms

As a class, ethers tend not to be very water soluble and have fairly low boiling points (although like hydrocarbons, very small amounts of ethers can be water soluble). However, just like the hydrocarbon functional group, molecules that contain the ether functional group are not very reactive. They have been used as fuel additives for automotive gasoline, and cause the octane rating to increase when added to gasoline. Examples include the oxygenated additive known as methyl-t-butyl ether (MTBE, $CH_3OC(CH_3)_3$), and the common solvent used in organic reactions, diethyl ether ($CH_3CH_2OCH_2CH_3$) as shown in Fig. 3.7.

Alcohol In another arrangement of carbon, hydrogen, and oxygen, the oxygen atom is attached to a carbon on one side and a hydrogen on the other. The result is the alcohol functional group. Yes, that is the same arrangement that we find in ethanol (CH_3CH_2OH), the alcohol in beer. Keep in mind, however, that formally, the word "alcohol" is just a word that tells us the arrangement of atoms in the

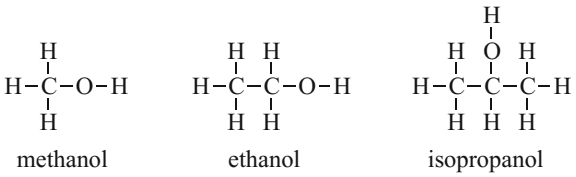


Fig. 3.8 The structure of some common alcohols

molecule. While the word "alcohol" is often used as the common name for ethanol, it is a functional group name. There are many compounds that have the alcohol functional group, such as methanol (CH_3OH), isopropanol (rubbing alcohol, $(CH_3)_2CHOH$), and even glucose ($C_6H_{12}O_6$). As a class, the alcohols tend to be somewhat soluble in water and have very high boiling points. Unlike the ethers and hydrocarbons, alcohols have the ability to react with a wide variety of chemicals to make other compounds.

Ethanol is a small molecule that is infinitely soluble in water and has a boiling point of 78 °C. This does not seem like a very large boiling point, but comparing ethanol to propane (a molecule with about the same mass), it is much larger. Propane's boiling point is −188 °C.

Ketone In another arrangement, the oxygen could have two attachments to the same carbon atom. This results in a double bond between the carbon and the oxygen atom in the molecule. This arrangement gives rise to a class of molecules known as a ketone (pronounced KEY-tone). Ketones have boiling points and solubility in water that is very similar to the ether functional group (small ketones tend to have some solubility in water, larger ones tend not to be very soluble). However, ketones are significantly more reactive than ethers. The ketone functional group is found in many common molecules, such as acetone (CH_3COCH_3), methyl ethyl ketone (MEK, $CH_3COCH_2CH_3$), and in more complex molecules such as fructose ($C_6H_{12}O_6$) as shown in Fig. 3.9.

Aldehyde Afunctional group related to the ketone is the aldehyde. This functional group requires a double attachment of an oxygen to a carbon atom, but also requires that the carbon atom be attached to another carbon and a hydrogen. The aldehyde

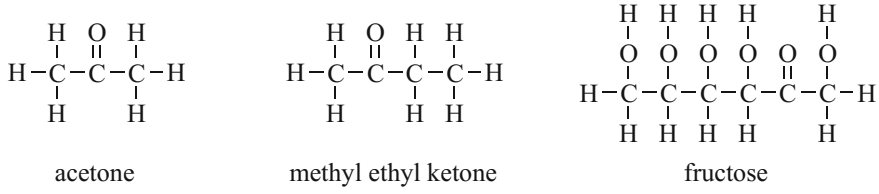
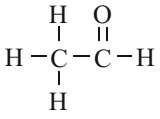


Fig. 3.9 Some common ketones. Note that every carbon still has four bonds and every oxygen still has 2 bonds



acetaldehyde

Fig. 3.10 Acetaldehyde contains the aldehyde functional group

functional group is common in carbohydrates such as glucose. Aldehydes have physical properties such as solubility and boiling point that are very similar to the ketones. However, the aldehydes tend to be fairly reactive. They are noted to undergo oxidation in air very easily. A common off-flavor in beer results from the presence of acetaldehyde, also known as ethanal (Fig. 3.10). Note the similarity of ethanol and ethanal.

Ester Another arrangement of oxygen into a carbon-containing molecule is known as the ester. This arrangement of atoms requires two oxygen atoms—one arranged in a similar fashion as an ether, and one arranged like a ketone (see Fig. 3.9). It is important that both oxygen atoms are attached to the same carbon atom, otherwise the functional group is not an ester. Such a molecule would contain two functional groups, the ether and the ketone.

The result is a somewhat water-soluble compound that has an intermediate boiling point. In other words, the solubility in water is about half that of the alcohols and the boiling point is somewhere between the alcohols and ketones. The most interesting feature of molecules containing the ester functional group is that they tend to have a pleasant fruity odor. Examples of molecules containing this group include methyl formate, ethyl acetate, and isoamyl acetate. Methyl formate (boiling point 32 °C) has a strong plum-like odor and flavor, ethyl acetate (boiling point 77 °C) has a solvent odor and flavor, octyl acetate (boiling point 211 °C) has a distinct orange odor and flavor, and isoamyl acetate (boiling point 142 °C) has the taste and odor of banana (see Fig. 3.11).

In brewing, the esters play a very large role in the flavors of the finished product. Many are made in only very tiny quantities, but the strength of their flavor and odor are easily detected by the tongue and nose. For example, isoamyl acetate can be detected as low as 1.1 parts per million. This is equivalent to being able to taste one drop of flavor in 14 gallons of water.

Carboxylic Acid Another functional group containing two oxygen atoms and one carbon atom is closely related to the ester functional group. It differs from the ester functional group in that the combination of a ketone and an alcohol form the carboxylic acid. They tend to be fairly soluble in water and have relatively high boiling and melting points. But the most important property of the carboxylic acids is that they are acidic. When dissolved in water, the carboxylic acid functional group dissociates into an H^+ ion and the carboxylate anion. This causes the pH of

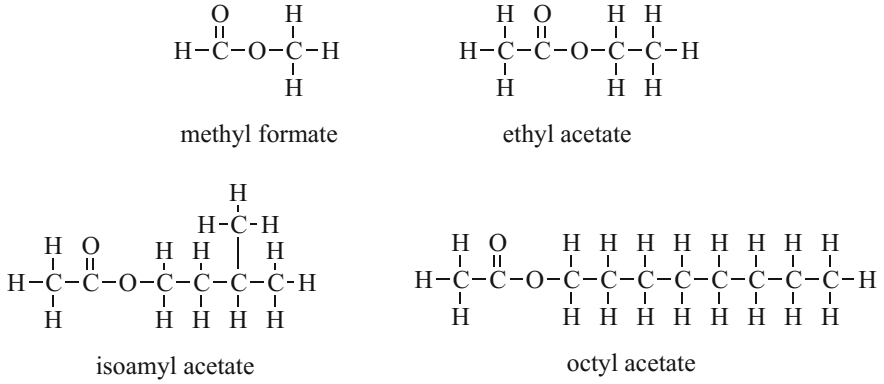


Fig. 3.11 Some esters

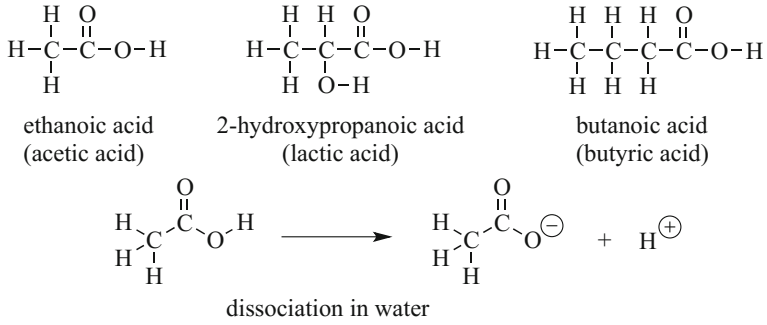


Fig. 3.12 Some common carboxylic acids and the dissociation in water

the water to drop. While not as acidic as hydrochloric acid, the carboxylic acid is still an acid.

One of the important organoleptic properties of the carboxylic acids is that they have a sour taste and odor. For example, acetic acid is better known as the acid used in making vinegar (a 10 % solution of acetic acid). Lactic acid and butyric acid are other examples of carboxylic acids. Figure 3.12 lists the structures of these compounds.

Amine The amino functional group is also encountered in brewing. This functional group contains a nitrogen atom attached to a carbon or hydrogen atoms. While the functional group does occur by itself in common organic molecules such as propanamine, the most common occurrence of the functional group in brewing is when it is combined in a molecule that already contains the carboxylic acid functional group. The result is the amino acid. Figure 3.13 lists an amine and an amino acid.

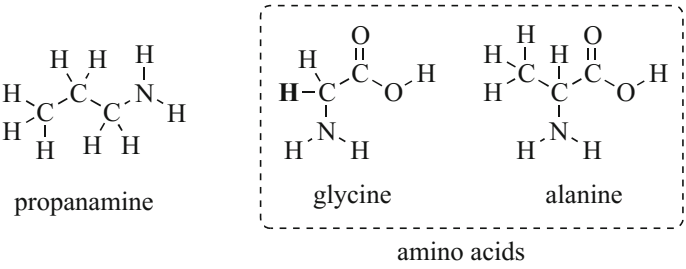


Fig. 3.13 Amine and amino acids. There are 20 amino acids used in the human body, only two are represented here. Each differs in the group that replaces the bold hydrogen in glycine

CHECKPOINT 3.4
Identify the different functional groups found in carvone (Fig. 3.3).
How many bonds do H, C, N, and O prefer in an organic molecule?

3.3.2 Amino Acid Polymers

A polymer is a molecule made up from a series of repeating smaller molecules. As we will discover as we explore mashing, a very common naturally occurring polymer is starch. Starch, a very large molecule, is made up of glucose molecules attached together in a repeating fashion. In this example, starch is the polymer and glucose is the monomer. Cellulose is another example of a polymer made up of glucose monomers attached in a different configuration. DNA is a polymer made from nucleic acid monomers.

For the brewer, another important polymer arises from the combination of amino acids. The resulting polymer is known as a peptide if there are only a small number of amino acids in the chain. If the chain is fairly long, the amino acid polymer is known as a protein. Yes, a protein is simply a chain of amino acids that are chemically bonded together. The protein is formed in the body using enzymes and biological mechanisms, but can be simply as shown in Fig. 3.14. The product is the formation of the peptide bond and the elimination of water.

The peptide chain results from the chemical reaction of the amino end of one amino acid and the carboxylic acid end of another amino acid. The result is the formation of the amide (pronounced "AM–id" in the USA) functional group that contains the C=O bond and a nitrogen atom attached to the C=O. The new bond that is formed (the C–N bond) is known as the peptide bond. This bond is very rigid and difficult to break. For these reasons, the amino acid functional group is very stable and the proteins tend not to react with water or other compounds.

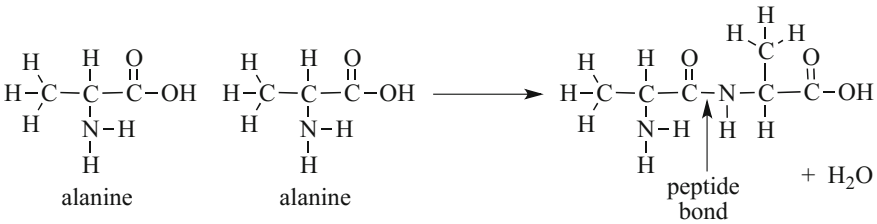


Fig. 3.14 The formation of the amide functional group in making a protein. The peptide bond in the amide functional group is noted

In some cases, the amino acid polymer aids reactions in the body or other biological system. The polymer in this case is known as an enzyme. On the surface, there is very little difference between a protein and an enzyme, other than the ability of an enzyme to aid the progress of other reactions. We will uncover a lot about enzymes and the reactions that they help catalyze later in this text.

CHECKPOINT 3.5
Write the product of the reaction of glycine with another glycine.
How many different molecules (not counting the water molecule) are formed if a glycine reacts with an alanine?

3.3.3 Drawing Organic Molecules

Thus far, we have looked at organic molecules by showing all of the atoms involved. Drawing these on paper take a very long time and if the molecule is sufficiently large, the clutter from showing every atom and bond makes it difficult to see the key structure or functional group in the molecule. A simpler way to draw these molecules exists, and it is the method we will use to represent organic molecules from this point forward.

The shorthand is known as line drawing. Successfully drawing a molecule using shorthand requires that we understand the number of bonds preferred by atoms such as carbon, nitrogen, oxygen, and the halogens (chlorine, bromine, iodine, etc.). In addition, it relies on our further understanding of the geometry of organic molecules.

For example, within a molecule is a collection of atoms, each with a nucleus. Those nuclei contain protons and neutrons and are positively charged. Because positive charges repel each other (just like two north pole ends of a magnet push apart), the atoms within a molecule push their nuclei to be as far apart as they can get. In other words, the atoms in a molecule do everything they can to be splayed out as far apart as possible.

The results are best represented by examples. For carbon, it is possible that it is attached to four other nuclei. In such a case, the carbon atom looks like a tetrahedron (and the angle between each adjacent nucleus is 109°). If the carbon participates in a double bond, then only three nuclei are attached. In that case, the best arrangement looks like the letter "Y" and the angles are 120°. If the carbon participates in a triple bond as it does in the alkyne functional group, then it is only attached to two other nuclei and is linear with bond angles of 180°.

Nitrogen prefers three bonds and in the functional groups common to the brewer, it adopts a shape that looks like a three-legged stool. The bond angles in this type of arrangement are 109°. Oxygen when it has two single bonds looks like the letter "V" with bond angles of 109°.

Thus, when we draw molecules using the shorthand, we try to show the 109°, 120°, or 180° angles. As you will see from the examples, it takes a little practice to get the drawings just right, but with that practice you will be able to draw the molecules much faster than by showing every atom.

The rules to drawing a line drawing of a molecule are very straightforward. First, any hydrogen that is attached to a carbon atom can be omitted from the drawing. If the hydrogen is attached to an oxygen or nitrogen, it must still be represented in the drawing. Second, all carbon atoms are not drawn. Third, only the bonds connecting each atom are represented and done so to reflect the bond angles.

Let us practice this by drawing the line drawing for ethanol (Fig. 3.8). We start by placing our pencil on the paper (i.e., the first carbon), then drawing a line (i.e., the second carbon), then pointing off at about 109° we draw a line to the oxygen. Finally, we add the oxygen and the hydrogen to the drawing (see Fig. 3.15).

Figure 3.16 shows a series of organic molecules and the line drawings that they represent. Note which atoms are omitted from the line drawings and also note the bond angles represented by the different structures. When performing the line drawings, it is very important to remember that even though some of the atoms are omitted, they are still there. This requires that we remember that carbon always makes four bonds, nitrogen makes three bonds, oxygen makes two bonds, and hydrogen and the halogens make only one bond.

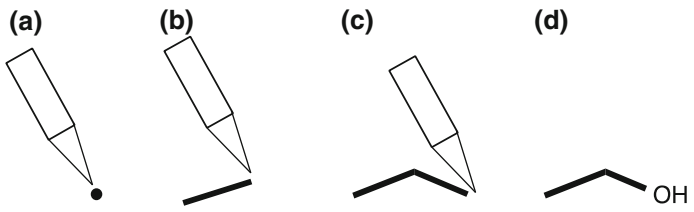


Fig. 3.15 How to draw a line drawing. We start with the pencil on the paper (**a**), draw a line to the next carbon atom (**b**), and finally to the oxygen atom (**c**). Then, we add the oxygen and hydrogen atoms to the drawing (**d**)

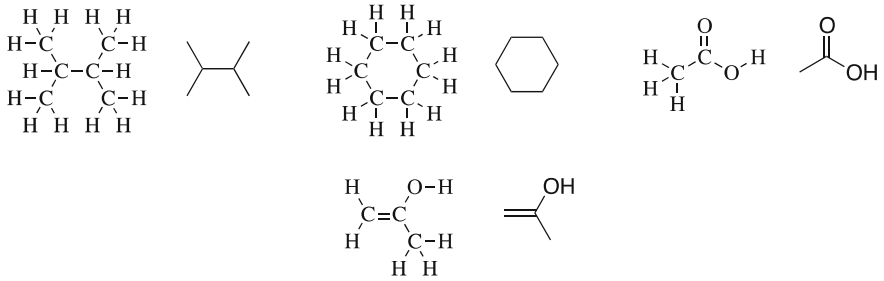
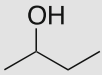


Fig. 3.16 Organic molecules and line drawings. Note the relationship between the fully expanded molecules and the simpler line drawings

CHECKPOINT 3.6
Rewrite the molecules in Fig. 3.5 using line drawings.
How many hydrogen atoms are there on each carbon in this line drawing?



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3.3.4 Naming Organic Molecules

While the average brewer will only be exposed to a couple hundred organic molecules (hop oils contain quite a few compounds), knowing how to systematically name the basic structures can provide a wealth of information on any molecule you might run into. Luckily, rather than being required to memorize the names of each of the million or so known organic compounds, the International Union of Pure and Applied Chemistry (IUPAC) has developed a set of rules to arrive at a molecule's name. These rules help us construct a name for a molecule if we know its structure. Unfortunately, many of the compounds in the brewery were identified and named before conventional rules were developed. We will introduce those names as well, but will focus on the use of the IUPAC nomenclature to identify these compounds.

Table 3.5 lists the basic steps in writing a name for a molecule. Consider we wish to provide the name of the compound shown here:

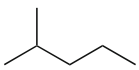
Let us use Table 3.5 to arrive at its name. First, we identify the functional group for the molecule (this compound is an alkane). Then, we count the longest chain of carbon atoms in the molecule. Using this, we write "pent" and add the ending for

Table 3.5. Rules for naming organic molecules

1	Identify the functional group and the ending for the molecule			
	alkane	ane	alkene	ene
	alkyne	yne	alcohol	ol
	ketone	one	aldehyde	al
	ester	ate	carboxylic acid	oic acid
2	Count the longest carbon chain and determine the name for that length			
	1	meth	6	hex
	2	eth	7	hept
	3	prop	8	oct
	4	but	9	non
	5	pent	10	dec
3	Combine the functional group ending with the longest chain name. Often, two or more functional groups exist. Add both endings to the longest chain name			
4	Number the chain to give the functional group (or branch) the smallest number. The functional group should always have the smallest number			
5	Add the functional group to the end of the molecule name with its number			
6	Add the branch name to the front of the molecule with its number			
	Branches are named using Rule #2, but end in "yl"			

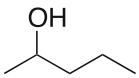
the functional group "ane" to arrive at the name "pentane." This method works very well for simple unbranched molecules.

For molecules that have a branch, we would then add the branch to the name. For example, consider that we have the molecule shown here:



We start by identifying the functional group (Rule #1). Here, again, this is an alkane. We count the longest carbon chain and arrive at pentane again (Rule #2, 3). However, this molecule has a branch. So, we number the carbon atoms to give the branch the lowest number. Then, we identify the group and add that, and the number, to the front of the name. The result here is 2-methylpentane.

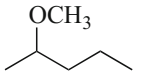
If the functional group is not an alkane, then we must identify the carbon in the molecule that contains the functional group. Consider the molecule here as we name it:



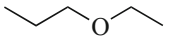
We start by recognizing this is an alcohol and an alkane. Then, we write the name for the longest carbon chain (pent) and add the functional group ending to the

molecule name (pentanol). We add the number of the carbon that contains the non-alkane group. The result is pentan-2-ol. Note that we dropped the "e" from pentane when we added the "ol."

Ethers are named differently from other functional groups. The oxygen atom in these molecules is considered to be part of a branch. The ending of the branch then becomes "oxy" instead of "yl." For example, the name of these ethers follows this rule:

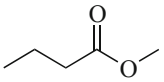


2-methoxypentane

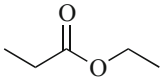


1-ethoxypropane

Esters are named very similarly to others, except that the group on the oxygen is placed in front of the name as a separate word ending in "yl." The rest of the rules apply. The names of some esters are shown here:

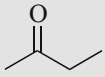


methyl butanoate



ethyl propanoate

CHECKPOINT 3.7
Name this molecule: $CH_3CH_2CH_2CH_2OH$
What is the name of this molecule?



3.4 Reactions of Organic Molecules

Hundreds of different chemical reactions take place during the brewing process. The most common of these are the reaction of organic molecules with water, with oxygen, and with other molecules. These reactions result in a large number of new molecules, each of which has a significant impact on the resulting beer. In many cases, the brewer anticipates these reactions. And the flavors, colors, and properties the products lend to the finished beer are desirable. In some cases, the reactions are not desirable. Such reactions result in negative impacts to the beer.

3.4.1 Oxidation and Reduction

Oxidation and reduction are the reactions that change the number of chemical bonds to oxygen atoms within a molecule. Reduction is the process that results in a decrease in the number of bonds to oxygen; oxidation increases the number of bonds to oxygen. The brewing process is an oxidative process. In the hop plant, during the boil, the mash, and other processes, oxidation reactions predominate. This is due to the presence of oxygen. The chemical reactions during yeast metabolism are also focused on oxidation processes that convert sugars into carbon dioxide and ethanol.

Consider the following chemical reaction that occurs during the fermentation process (Fig. 3.17). If we count the number of bonds between carbon atoms and oxygen atoms in the molecule on the left (the reactant), we see six individual attachments (two single bonds and two double bonds). In the molecules on the right (the products), there are eight bonds between carbon atoms and oxygen atoms (four double bonds). This is an oxidation reaction.

3.4.2 Condensation Reactions

Condensation reactions are also common in brewing. This reaction type involves the combination of two smaller molecules to give a larger molecule and a very small stable molecule. Typically, that smaller stable molecule is water (H_2O). Condensation reactions, as a rule, result in the formation of larger molecules.

Consider the reaction of acetic acid and ethanol shown in Fig. 3.18. In this reaction, two molecules are joined together to make ethyl acetate with the elimination of a water molecule. The condensation of a carboxylic acid and an alcohol results in the formation of an ester. While esters are commonly formed during yeast metabolism, the particular condensation that occurs to form most of those esters occurs using slightly different reactant molecules.

The reverse of this reaction is also possible during the brewing process. In such cases, an ester reacts with water to form the carboxylic acid and an alcohol. Any reaction that involves water and is the reverse of the condensation reaction is known as a hydrolysis reaction. Hydrolysis (or reaction that breaks a molecule with water) reactions are quite common in the boil where hot water under acidic conditions adds

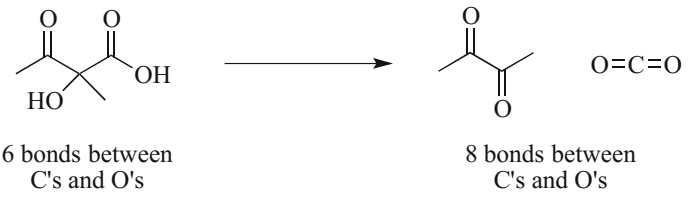


Fig. 3.17 The formation of diacetyl from alpha-acetolactate is an oxidation reaction

Fig. 3.18 The formation of an ester via a condensation reaction. Note the formation of water as one of the products

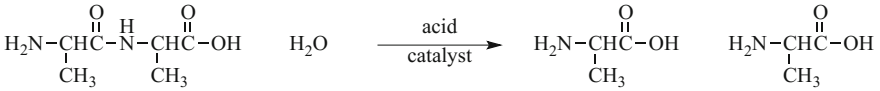


Fig. 3.19 Hydrolysis of a larger peptide or protein gives rise to the individual amino acids. Note that water is incorporated into the products

to molecules and breaks them into smaller compounds. The hydrolysis reaction is one way in which larger proteins are decomposed into their individual amino acids (see Fig. 3.19).

3.4.3 Isomerization Reactions

While there are not very many reactions of this type that occur in the brewing process, those that do take place are extremely significant. In the isomerization reaction, the structure of a single molecule becomes altered to form a new molecule. The new molecule ends up with properties that are different from the original molecule.

The best example of the isomerization reaction is the conversion of humulone (also known as α-acid) to isohumulone (also known as iso-α-acid) as shown in Fig. 3.20. Humulone is a molecule found in hop oil. During the boiling process, this molecule is converted via an isomerization reaction into the molecule that we associate with the bitter flavor of a hopped beer. In addition to the differences in the flavor of the two molecules, there is a notable difference in the solubility of the molecules in water; isohumulone is nearly twice as soluble in water compared to humulone.

3.4.4 Radical Reactions

There are some radical reactions that take place in beer. These reactions are difficult to detect by looking at the reactants and products because the name of this type of reaction comes from how the reaction occurs. In the radical reaction, a very-high-energy species is formed during the reaction. This species have high energy because it contains a single unpaired electron.

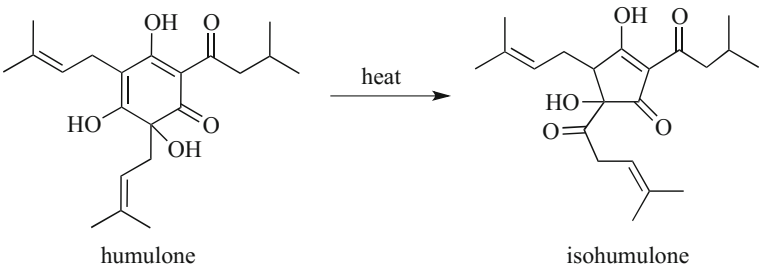


Fig. 3.20 The isomerization of humulone to isohumulone. Note that the number of atoms do not change in the reactant or product of the reaction, only the arrangement of the atoms changes

In the course of the reaction, the single electron is often formed by the interaction of a molecule with sunlight. In many cases, this is the only way to tell that the reaction involves radicals. A common example of a radical reaction is the formation of the skunk-like flavor in light-struck beer, see Fig. 3.21. Note that by only considering the reactants and products, it is very difficult to determine that this is a radical reaction.

The mechanism, or process by which the reaction occurs, does show the formation of radicals. As shown in Fig. 3.22, the actual process involves the activation of a protein in beer by light. The protein then causes isohumulone to become activated. That molecule then cleaves into two and eliminates a molecule of carbon monoxide, and the radical reacts with a sulfur atom on cysteine to make the skunk-flavored molecule.

CHECKPOINT 3.8
Outline the key parts of the four reaction types described here.
Write the reaction that describes the hydrolysis of ethyl acetate.

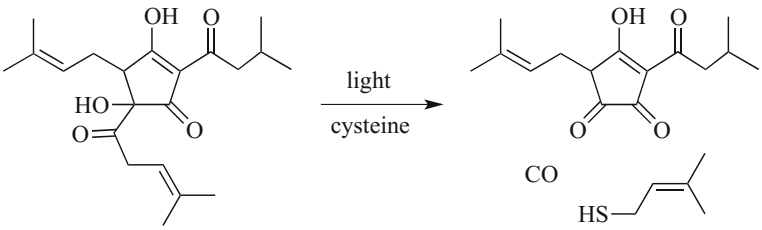


Fig. 3.21 The radical reaction of isohumulone with cysteine, an amino acid, forms the sulfur compound responsible for the skunk flavor in lightstruck beer

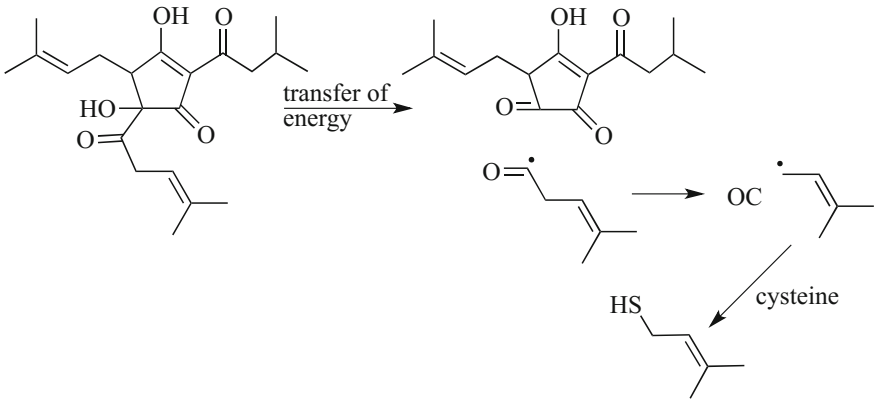


Fig. 3.22 The mechanism of the reaction of isohumulone with light. Note the formation of radicals in the formation of the sulfur-containing molecule

3.4.5 Maillard Reactions

If we take a spoon of sugar and heat it up, we notice some very interesting changes. First, the sugar melts, then starts to brown. If we continue heating the sugar, it begins burning and becomes charcoal-like. These are chemical reactions that are taking place, changing the sugar molecule into new molecules. Many of these new molecules result from the loss of water, condensation reactions, isomerizations, and a host of other reactions. Some of the possible compounds formed are shown in Fig. 3.23.

This process is known as caramelization, and the resulting flavors of the heated spoon of sugar reflect that. Initially, the flavors do not change much, but once the sugars turn brown the flavors of caramel, toffee, and eventually charcoal are noticeable. These flavors are due to the larger cyclic compounds that are made in the reaction. Note that these compounds only contain carbon, hydrogen, and oxygen atoms.

Chemists studied caramelization extensively. By the 1900s, the reactions of sugar with other molecules were being explored. During his study of what happened when amino acids and sugars were heated together in the laboratory, Louis Camille Maillard (pronounced "may-yar") noted a similar caramelization. However, the result was the formation of a complex mixture of products that, while similar to caramelization reactions, contained nitrogen (see Fig. 3.24). These reactions are known as Maillard reactions. Chemists and food scientists continue to study the mechanism of the Maillard reactions to learn more about the compounds that are formed.

Maillard reactions occur when most foods are cooked because of the presence of both sugars and proteins. When we brown toast or grill a steak, evidence of the

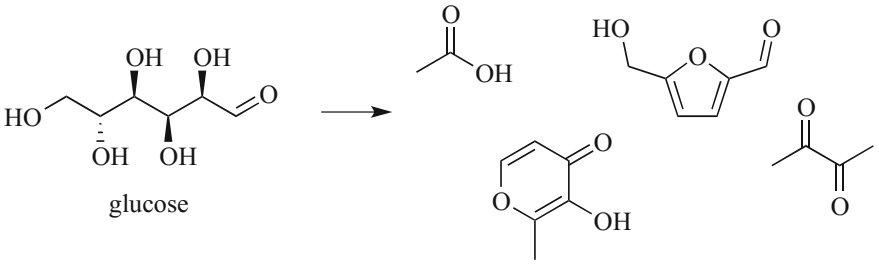


Fig. 3.23 Caramelization of sugar. This results in compounds containing oxygen, hydrogen, and carbon

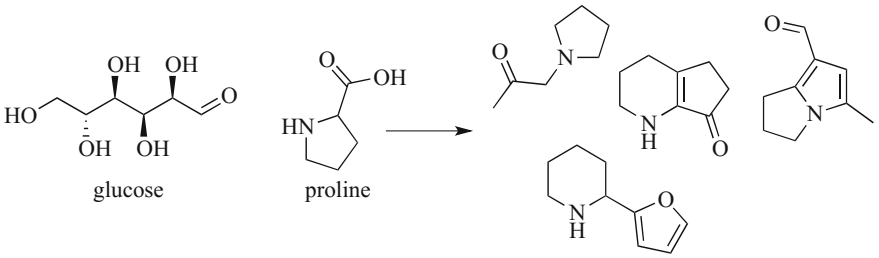


Fig. 3.24 The Maillard reaction of sugar and amino acids. Proline, an amino acid common in grain, is shown here. The products include those of the caramelization reaction (see Fig. 3.22), but also include cyclic compounds containing nitrogen

Maillard reaction appears as a brown color on the surface of the food. When malt is kilned, when wort is boiled, or when heat is added at any time during the brewing process, Maillard reactions occur. In fact, Maillard reactions occur anytime that heat, sugars, and proteins are found together.

While the mechanism of the reaction is rather complex, what is known is that the speed of the reaction between sugars and amino acids increases as the temperature of the heating process increases. If prolonged heating or high temperatures are involved, the amount of the Maillard products predominates. And with any increase in temperature, the caramel, toffee, toast, and other flavors become more and more noticeable. For example, the rich caramel and malty flavors of the bock style of beer result from the addition of heat during the mashing process (in a process known as decoction mashing).

The flavors of Maillard products are similar to those of caramelization. There is a slight difference in that the nitrogen-based compounds add an earthier, coffee-like tone to the flavors. In addition, these coffee-like flavors tend to appear earlier than in the absence of amino acids.

Chapter Summary

Section 3.1

All matter is made up of atoms.
How electrons are shared between atoms indicates the type of bond between those atoms.
Names for simple binary compounds have been developed.

Section 3.2

Laws and theories govern the rules of chemistry.
The laws and theories result in our understanding of how atoms are arranged in molecules.

Section 3.3

Molecules that contain carbon and hydrogen are classified as organic molecules.
Organic molecules may contain other nonmetals in addition to carbon.
The study of organic molecules is made easier by classifying them into functional groups, based on the arrangement of atoms in the molecule.
Line drawings are an easier way to represent organic molecules.
Rules for naming organic molecules exist.

Section 3.4

There are four main types of chemical reactions that occur in brewing.
Caramelization and Maillard reactions provide much of the toasty, caramel, toffee, and coffee flavors. These reactions also darken the color of the resulting beer.

Questions to Consider

1. Describe the hypothesis by Democritus in your own words.
2. According to Dalton's atomic theory, is it possible to convert lead into gold? Explain.
3. How many electrons, protons, and neutrons do F, S, Mg, B, and P have?
4. How many electrons do Na^{+}, N^{3-}, O^{2-}, and Cl^{-} have?
5. What is the likely formula for a compound made from boron and chlorine?
6. What is the likely formula for a compound made from lithium and oxygen?
7. What is the name for the compounds you described in #5 and #6?
8. What is the name for these compounds: CS_2, P_2S_3, N_2O_2, and ClO?
9. Draw all of the possible molecules with the formula C_5H_{12} and provide their names.
10. Draw all of the possible alcohols with the formula $C_4H_{10}O$ and provide the name of each.

11. Draw all of the possible compounds containing a C=O with the formula $C_5H_{10}O$ and name each one.
12. An ester has 4 carbon atoms. Draw all possible esters that satisfy this statement and name each one.
13. Show the condensation reaction that would provide each of the esters you drew in #12.
14. Based on your understanding of oxidation and reduction, arrange the oxygen-containing functional groups in order of their oxidation state (most oxidized first).
15. An amide is formed between propanamine (see Fig. 3.13) and a 2 carbon carboxylic acid. Draw the condensation reaction of this reaction.
16. Explain, in your own words, the difference between a caramelization reaction and a Maillard reaction.
17. Using your own experience, explain the law of conservation of mass.
18. The reaction of butane with gaseous oxygen (O_2) produces carbon dioxide and water. Write this reaction out and balance it to make sure the number of atoms is the same on both sides.
19. In Fig. 3.23, one of the compounds identified as a product of the reaction is a carboxylic acid. Name it and propose a flavor for the compound.
20. Draw and name all of the ethers with the formula $C_4H_{10}O$.
21. What is the functional group in the molecule diacetyl? Propose a chemical name for this molecule.

Laboratory Exercises

Building Models in 3-D

This "experiment" is designed to familiarize you with the shapes of different molecules that you might encounter in the science of brewing. Organic molecules are not flat; they have a 3-D shape based on the number of atoms that are attached at each location in the molecule.

Equipment Needed

Organic chemistry model kit—containing a minimum of 6 carbons, 12 hydrogen, 6 oxygens, and 1 nitrogen atom.

Experiment

In this experiment you will build models of each of the following molecules, draw a diagram of what you have built and then answer the questions about each model you have built.

CH_4—describe the shape of this molecule in your own words.
H_2O—does the shape of this molecule have a comparison to CH_4?

NH_3—compare the shape of this molecule to water and methane (CH_4).
C_2H_4—describe the shape of the carbon atom in this molecule.
C_2H_2—describe the shape of the carbon atom in this molecule. Is there a trend between CH_4, C_2H_4, and C_2H_2?
CH_3CH_2OH—is there a relationship between the atoms in this molecule and the separate molecules of CH_4 and H_2O?
C_5H_{10}—build a molecule that is cyclic. How many different molecules can you make?
C_5H_{12}—build a linear version of this molecule. When stretched out as far as possible, describe the shape of the carbon chain.
$C_4H_{10}O$—how many different molecules can you construct? Be sure to account for stereochemistry.
$C_6H_{12}O_6$—build a cyclic molecule containing 1 oxygen in the ring. This is a carbohydrate. Notice that there are many different options for arranging this molecule. Assuming that you place 5 carbons and 1 oxygen in the ring, how many different arrangements of the remaining atoms are there?