CHEMISTRY
CHALLENGES AND SOLUTIONS

Unit 6: *Quantifying Chemical Reactions—Stoichiometry and Moles*

Unit Overview

Elements combine in definite ratios, and the results of a chemical reaction can be predicted using balanced chemical formulas along with careful measurements of the amount of reactants. In this unit, we will explore atomic mass, the limiting reactant (the first reactant to be used up), and the yield of a reaction. Quantification of chemical reactions is key to all the practical applications of chemistry, from developing new energy resources to chemical manufacturing.

by Adam Brunet

Sections

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Unit 6: *Quantifying Chemical Reactions—Stoichiometry and Moles*

Section 1: Introduction

Chemists make many detailed observations about how matter behaves. To represent this information, they use formulas that summarize chemical reactions with numbers and symbols. As Figure 6-1 shows, chemical formulas make it possible to describe complex processes very concisely.

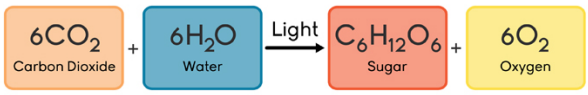


Figure 6-1. Chemical Formula for Photosynthesis

Photosynthesis is the process by which plants turn carbon dioxide from the atmosphere into carbohydrates (plant tissue), using light as an energy source and releasing oxygen as a byproduct. Photosynthesis is one of the most important biological processes on Earth: It makes air breathable, and supplies most of the energy required for all life forms.

In this unit, we will learn how to use chemical formulas to summarize what we know. Important types of chemical formulas include:

- Empirical formulas, which describe the ratios in which elements combine to form compounds;
- Molecular formulas, which show the numbers of different atoms in these compounds; and
- Lewis structures, which symbolize the bonds between the atoms from the formulas that give compounds their unique properties.

Using the process of combustion analysis (burning a material to break it into its component parts so that we can determine its makeup), we will see how chemists use formulas to summarize laboratory experiments. To describe activities such as combustion analysis accurately, chemists use specific terms to measure mass and volume. We will learn about moles, Avogadro's rule and number, atomic mass, molecular mass, and how to find mass percentages for molecules and mixtures. Finally, we'll want to see what happens when we put different compounds together in chemical reactions. We'll look at how we balance a chemical equation, equilibrium reactions, limiting reagents, and yields.

Stinking Up the House

As a boy in London during World War II, neurologist and author Oliver Sacks was fascinated with chemistry. Here, he describes an experiment that worked too well.

I had smelled a bit of hydrogen sulfide in Uncle Dave's lab—it smelled of rotten eggs and farts and (I was told) volcanoes. A simple way of making it was to pour dilute hydrochloric acid on ferrous sulfide. (The ferrous sulfide, a great chunky mass of it, I made myself by heating iron and sulfur together till they glowed and combined.) The ferrous sulfide bubbled when I poured hydrochloric acid on it, and instantly emitted a huge quantity of stinking, choking hydrogen sulfide. I threw open the doors into the garden and staggered out, feeling very queer and ill, remembering how poisonous the gas was. Meanwhile, the infernal sulfide (I had made a lot of it) was still giving off clouds of toxic gas, and this soon permeated the house. My parents were, by and large, amazingly tolerant of my experiments, but they insisted, at this point, on having a fume cupboard installed and on my using, for such experiments, less generous quantities of reagents.

Oliver Sacks, *Uncle Tungsten* (2001), pp. 89–90.

Quantifying chemical processes accurately is critically important in the chemical industry and related fields, such as pharmacology (developing and manufacturing drugs). To produce substances that consistently have the required qualities, and to do so efficiently and cost-effectively, chemists need to know exactly how much of every reagent (ingredient) goes into a reaction, and how much of what types of substances will be produced. When scientists know exactly what processes will happen in a reaction and how much of each reagent they will need, they can avoid ending up with large quantities of expensive materials left over. They can also avoid making too much product, as renowned neurologist and author Oliver Sacks did in a boyhood chemistry experiment. (See *Stinking Up the House* sidebar.)

Unit 6: *Quantifying Chemical Reactions—Stoichiometry and Moles*

Section 2: Empirical and Molecular Formulas

Empirical Formula

As we saw in Unit 1, scientists started analyzing the general ratios in which substances combined with each other in the 18th century. The simplest way to describe these ratios is with an empirical formula, which uses whole numbers to show how many atoms of each element make up one molecule of a compound. For example, the empirical formula of water is H_2O, which means there are two atoms of hydrogen for every one atom of oxygen in one molecule of water. (The subscript number always refers to the element just before it, and if no subscript is specified, then there is just one of that atom.)

Berzelius and the Birth of Formulas

Portrait of Jöns Jacob Berzelius. © Wikimedia Commons, Public Domain.

It wasn't until the early 1800s that scientists agreed upon a way to write down the contents of molecules in a consistent and formulaic way. This first form of chemical notation was developed by one of the fathers of modern chemistry, Swedish chemist Jöns Jacob Berzelius (1779–1848). Berzelius described this method for writing empirical and molecular formulas in an 1814 paper. When we look at the paper, it is curious to see that at first, chemists used superscripts (for example, SO^3 for sulfuric acid anhydride) instead of subscripts (for example, SO_3). This changed later due to the obvious confusion with mathematical operations.

Different elements can have the same empirical formula because it represents the lowest common denominator of the elements in a substance. For instance, both acetylene (C_2H_2), a compound used in welding torches, and benzene (C_6H_6), a carcinogenic industrial solvent, can be reduced to CH. For every atom of carbon, there is one atom of hydrogen in each molecule of each of these substances. An empirical formula only describes the ratio of atoms in a compound, not the absolute number of atoms.

Combustion Analysis

In the early 1800s, French chemist Joseph Gay-Lussac, whom we met in Unit 2, developed the process of combustion analysis as a way to calculate the ratio of atoms in organic compounds. When a compound burns, its chemical bonds break and each atom combines with oxygen in a gaseous form. By capturing and measuring these different gases, scientists can calculate the empirical formula of the original substance. This process is illustrated in Figure 6-2.

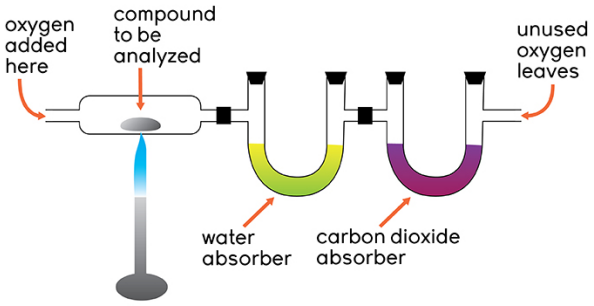


Figure 6-2. Combustion Analysis Setup

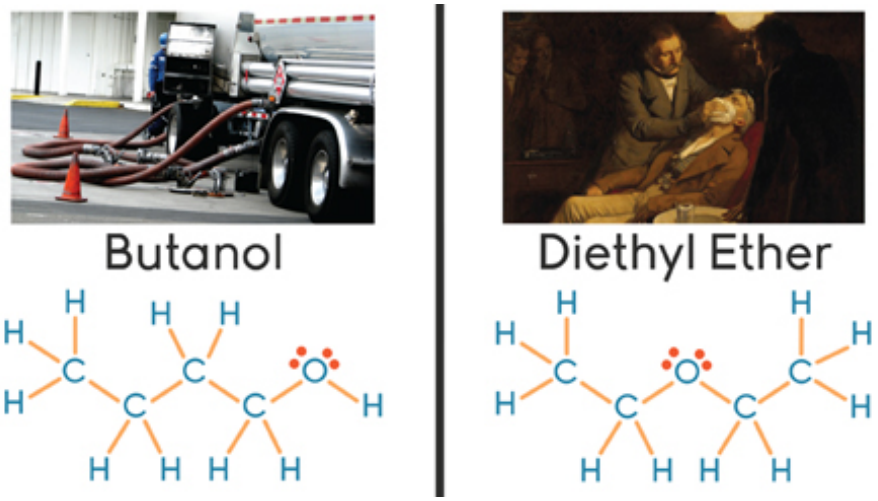
In a combustion analysis, burning a test compound breaks it into its component elements, which combine with oxygen from the surrounding air to produce various gases. Here, carbon in the material combines with oxygen to make carbon dioxide (CO_2), and hydrogen combines with oxygen to make water vapor (H_2O). These gases are collected by passing them through substances that trap each gas product separately. By weighing these absorbers, researchers can calculate how much of each gas was produced, and then deduce the empirical formula of the test compound.

For example, if we burn table sugar (the molecule sucrose, $C_6H_{12}O_6$), we'll produce the same amount (volume of gas) of carbon dioxide (6 molecules of CO_2) and water vapor (6 molecules of H_2O). Each water vapor (H_2O) molecule contains two hydrogen atoms and each carbon dioxide (CO_2) contains only one carbon. Since we have equal quantities of both gases, we know that the starting compound must have contained twice as many hydrogen atoms as carbon atoms. We can also carefully track the amount of oxygen that was added to burn the sucrose and the amount that remained after the process. Subtracting the quantity of oxygen remaining from the amount that was added tells us the number of oxygen atoms in the sugar.

At the end of it all, we will have determined the *relative* amounts of carbon, hydrogen, and oxygen in the compound. In sucrose, for every carbon atom there are two hydrogen atoms and one oxygen atom. This information is used to describe the sugar molecule by its empirical formula, CH_2O. These ratio numbers appear in the empirical formula as subscripts, $C_1H_2O_1$, but we don't usually write the "1": When no subscript is given, it is understood to be one.

Isomers and Lewis Structures

When two compounds contain the same elements in the same proportions but with different structures, these materials are called "isomers." If compounds A and B are isomers, a molecule of A and a molecule of B contain the same number of atoms of each type, but the bonds connecting these atoms are arranged differently. This seemingly subtle difference can produce compounds with dramatically different physical and chemical properties.



Butanol and Diethyl Ether. © Left: Wikimedia Commons, Public Domain, 2008. Right: Wikimedia Commons, Public Domain, 2007. Graphics: Science Media Group.

For example, butanol and diethyl ether have the same molecular formula ($C_4H_{10}O$). Because butanol has a hydrogen bound to its oxygen, it can hydrogen bond, which means it has stronger intermolecular forces, and thus a higher boiling point than the diethyl ether. At room temperature, butanol is a liquid that burns and is often used as an alternative to gasoline. Diethyl ether is also highly flammable, but just above room temperature it will vaporize into a gas, while butanol remains a liquid until 118°C. Inhaling butanol fumes can cause eye, nose, and throat irritation, but diethyl ether was widely used as an inhalation anesthetic from the mid-19th century through the early 20th century.

To understand why these two isomers have such different properties, we need a version of a formula that illustrates their different chemical bond arrangements. The best example of this is the Lewis structure, which was the focus of Unit 5. By expanding out all of the atoms so that we can see how many there are and how they are connected together, the properties of the molecules can be better understood. However, Unit 6 will be focusing on the properties of chemical reactions where only the molecular formula needs to be known.

Molecular Formula

The empirical formula tells us the correct ratio of atoms (6:12:6 is the same as 1:2:1), but not necessarily their actual numbers. A molecule of sucrose actually has 6 carbon atoms, 12 hydrogen atoms, and 6 oxygen atoms, 6:12:6. If we update the formula so it contains the actual number of atoms of each type, it is called the "molecular formula"; the molecular formula for sucrose is written $C_6H_{12}O_6$.

We can get from the empirical formula to the molecular formula if we know the mass of one molecule of sucrose. Then we can check whether it is equal to the mass of one carbon atom plus two hydrogen atoms plus one oxygen atom, or some larger multiple of that. The masses of molecules will be discussed later in this unit.

Unit 6: *Quantifying Chemical Reactions—Stoichiometry and Moles*

Section 3: Counting Particles—Moles

How Many Items Are in a Mole?

"Chemistry students have long amused themselves by computing just how large [a mole] is, so I can report that it is equivalent to the number of popcorn kernels needed to cover the United States to the depth of nine miles, or cupfuls of water in the Pacific Ocean, or soft drink cans that would, evenly stacked, cover the Earth to a depth of 200 miles. An equivalent number of American pennies would be enough to make every person on Earth a dollar trillionnaire."

Bill Bryson, *A Short History of Nearly Everything* (2003), p. 105.

Chemical formulas describe individual molecules, but scientists work with much larger quantities in the laboratory. A single molecule of water weighs 0.000000000000000000000000299 grams and occupies about 0.000000000000000000000000109 milliliters, so manipulating it would be challenging, to say the least! We simply don't have the ability to easily measure such small masses or volumes. Instead, we deal with particles (atoms, molecules, or ions) in large groups so that we can easily measure them. It is useful to have a standard size for these groups.

Figure 6-3. Amedeo Avogadro (1776–1856)

This great Italian scientist made important contributions to molecular theory, particularly Avogadro's Law. He began as a lawyer, and his interest in math and physics led him to become the first physics professor in Italy in 1820. It is in his honor that the number of objects in a mole is called "Avogadro's Number."

When we buy eggs at the supermarket, they come in groups of a dozen, which is considered a convenient number of eggs. In the same way, chemists decided more than a century ago that they needed a convenient number for the particles with which they worked. Because molecules were so small, that number had to be large.

The standard unit that chemists use for measuring large quantities of very small particles, such as atoms or molecules, is the mole (abbreviated as mol). One mole of any substance contains the same number of particles: 6.02214×10^{23}. A mole is a very large quantity (see *How Many Items Are in a Mole?* sidebar), but a mole of particles is just about the right amount of substance to look at easily in the laboratory.

Avogadro's Law Example

Balloons Filled with Helium (Left) and Carbon Dioxide (Right) © Science Media Group.

To see how scientists used Avogadro's Law, imagine filling a balloon with helium (He) to a certain volume, then filling a second balloon with carbon dioxide (CO_2) to the same volume. Both balloons must be at the same pressure and temperature, but that will be true if they are in the same room at the same time. According to Avogadro's 1811 theory, the number of helium atoms in the first balloon would be equal to the number of carbon dioxide molecules in the second balloon. This was an extraordinary insight and not at all obvious: Different gases are composed of particles with different masses and sizes. The fact that a given volume of any gas has the same number of particles is counterintuitive, but true. It allows us to establish that one gas has more mass than another, and 19th-century scientists were able to find the relative masses of each element and each compound to each other using this law. For example, if we were to find the mass that each balloon gained when they were filled, we would find that the mass of carbon dioxide is 11 times larger than the mass of helium in the other balloon. Thus, we can conclude that a molecule of carbon dioxide has a mass that is 11 times that of a helium atom.

This distinctive quantity is known as "Avogadro's number," named for Italian chemist Amedeo Avogadro, whom we met in Unit 2. Recall that in 1811, Avogadro theorized that equal volumes of gases under a constant temperature and pressure contained the same number of particles, regardless of what types of gases they were. His proposal was largely ignored for decades, but gained acceptance by the late 1850s. Other scientists used Avogadro's theory to determine atomic and molecular masses. The specific value of 6.02214×10^{23} was determined by Nobel Prize-winning physicist Jean Baptiste Perrin (1870–1942) in 1909. Perrin suggested that this number be named in honor of Avogadro.

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Section 4: Avogadro's Number and Atomic Mass

Early chemists defined the mole as the number of hydrogen atoms in one gram of hydrogen because that was the most accurate measurement they could make at the time. Later, because it was easier to obtain the ratio of atomic masses for most elements with oxygen than it was with hydrogen (for technical reasons), many people used oxygen as the standard for atomic masses. One mole was defined as the number of atoms in 16 grams of oxygen. The current standard for Avogadro's number was set in the 1960s to be the most precise one agreed on by chemists and physicists. We now define a mole in terms of carbon-12, the most common isotope of carbon, which has six protons and six neutrons in its nucleus. (We will cover more about isotopes of various elements in Unit 4 and Unit 12). One mole is the number of carbon-12 atoms in exactly 12 grams of carbon-12. From this new standard, precise measurements of all the atomic masses can be made and then extended out for compounds, as we will see in the next section.

If we remember, a dozen is a good metaphor for the mole; so let's consider a dozen eggs. One dozen chicken eggs and one dozen quail eggs—both have twelve eggs, but very different masses. For example, a dozen chicken eggs has a mass of 720 grams, while a dozen quail eggs has a mass of 96 grams. We can extend this to the mole. One mole of carbon-12 atoms has a mass of exactly 12 grams, but another type of atom will have a very different mass if we count out a mole of them. For example, a mole of gold atoms would have a mass of 197 grams.

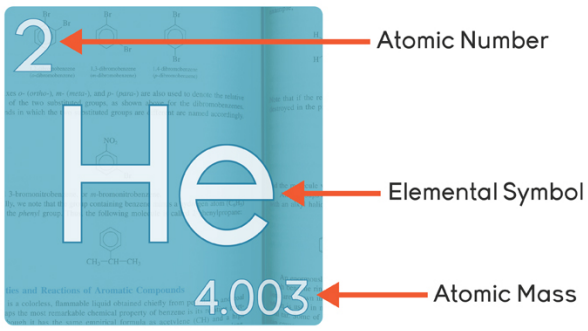


Figure 6-4. Finding the Atomic Mass on the Periodic Table of Elements

On the periodic table, the elements are ordered by their atomic numbers, which is the number of protons that particular atom has in the nucleus. Atomic mass is the average mass of atoms of an element, calculated using the relative abundance of isotopes in a naturally occurring element. In the case of helium, it is designated as 4.003 and is shown in the bottom right-hand corner.

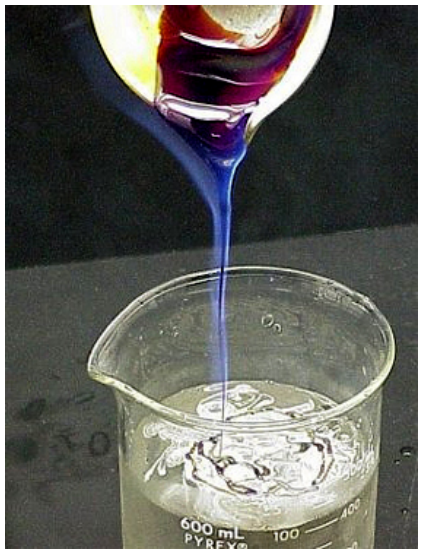
Avogadro's number makes it possible for us to convert an almost uncountable number of atoms or molecules into measurable amounts that can be determined as a mass by a scale. Since chemists have established that a mole of carbon-12 atoms has $6.02214179 \times 10^{23}$ atoms and an atomic mass of 12

grams, they calibrate mass spectrometers (instruments used to measure the very precise masses and relative amounts of atoms and molecules) to the mass of carbon-12. A mole of any other substance also contains 6.02×10^{23} atoms, but has a mass of more or less than 12 grams.

As we saw in Unit 4, each element in the periodic table has an atomic mass in the lower right corner, which represents the average atomic mass of all of the isotopes of that element. (Figure 6-4) Helium's atomic mass, or the average mass of a single atom of helium, is 4.003. Normally in chemistry, we make sure to write the units next to any numerical value we want to talk about. So, why is there not a unit next to the 4.003 for helium? Because there are actually two different ways to interpret that number, both of which are linked to the mole and Avogadro's number.

Converting Moles to Atomic Mass

So, how can people who want to learn chemistry use these atomic masses to figure out how much of an element they want? There are two common ways. Let's consider this. We need one mole of sulfur in order to make plastic sulfur, which is what happens when sulfur is melted and then poured into water. On the periodic table, we find that sulfur has an atomic mass of 32 g/mol. So, if we want one mole of sulfur, we should use a scale and get 32 grams of it.



Plastic Sulfur. © Charles Ward.

The other situation is when someone hands us 24 grams of sulfur and asks how many moles of sulfur we have. We can use that atomic mass to convert the grams of sulfur into moles of sulfur just by dividing:

$$\frac{24 \text{ grams of sulfur}}{(32 \text{ g/mol sulfur})} = 0.75 \text{ moles of sulfur}$$

Which can even be written out in words as:

mass/atomic mass = moles

Or can be written with multiplication as:

mass = moles X atomic mass

No matter how we think about masses and moles, so long as we have a periodic table with atomic masses on it, it is straightforward to convert back and forth between the mass of an element and the number of atoms of that element that are present.

So the number 4.003 technically means that if a carbon-12 atom has a mass of exactly 12, then a helium atom (on average) has a mass of 4.033. One way to interpret that number is in atomic mass units (abbreviated as u). An atomic mass unit is a very small unit of mass, about 1.66×10^{-27} kilograms. But talking about the masses of individual atoms is not very useful for trying to quantify chemical reactions. The other way to interpret that number on the periodic table is to say that it has units of grams per mole or g/mol. This means that on average a mole of helium atoms has a mass of 4.003 grams.

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Section 5: Molecular Masses and Mass Percentages

While masses are useful for individual atoms, most of the chemistry in the world around us is taking place between compounds that contain more than one atom and usually several types of atoms. For this purpose, we need to be able to come up with masses for molecules and compounds as well.

Molecular Mass

Since we know the atomic mass of individual atoms, we can figure out the molecular mass (or molar mass) of molecules composed of several atoms. Let's look at water. The molecular formula of water is H_2O. This means that each molecule of water contains one atom of oxygen (16 g/mol) and two atoms of hydrogen (1 g/mol for each atom). So a *mole* of water molecules has the same mass as the sum of the atomic masses of its components (18 g/mol). (Table 6-1)

Table 6-1. Find the mass of atoms in one mole of H_20:

16 g (1 mole of oxygen at 16 g/mol) + 2 g (2 moles of hydrogen at 1 g/mol each)
= 18 g (1 mole of water at 18 g/mol)

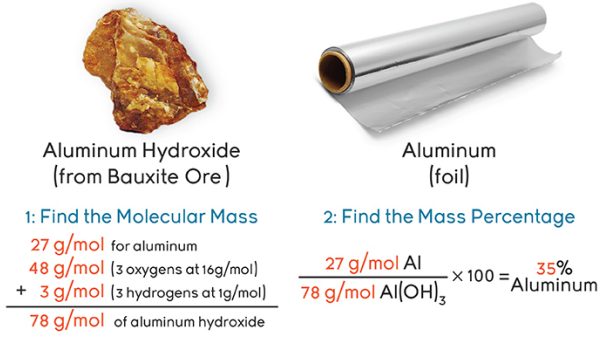

Figure 6-5. Mass Percentage of Aluminum in Aluminum Hydroxide

The molecular formula gives us the number of each type of atom in a molecule, but we can also discuss the composition of a molecule in terms of how much of its mass is contributed by each atom type. We call this the "mass percentage" of a given atom type in a particular compound.

Molecular Mass Percentages

The molecular formula gives us the number of each type of atom in a molecule, but we can also discuss the composition of molecules in terms of the fraction of its mass that is contributed by each atom type. We call this the "mass percentage" of a given atom type in a particular compound.

The formula is:

$$\text{Mass \% of Element A} = \frac{\text{Mass of element A in the molecule}}{\text{Mass of the whole molecule}} \times 100$$

Figuring out the mass percentage of an element is very important in many fields, including mineral extraction. Take aluminum (Al) as an example. Most of the world's aluminum is found in the form of the bauxite ore, which is composed mainly of aluminum hydroxide, $Al(OH)_3$. In order to extract the aluminum, we have to separate it from the oxygen and hydrogen. But how much aluminum will we get out of one kilogram of aluminum hydroxide? We find this by calculating the mass percentage. (Figure 6-5)

If we had one kilogram of aluminum hydroxide, we could expect to purify no more than 35% of it, or about 350 grams, into pure aluminum (Al).

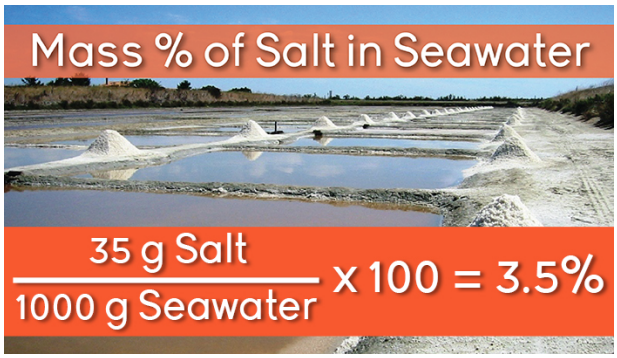

Figure 6-6. Mass Percentage of Salt in Seawater

Sea salt can be easily made by letting artificial ponds like these fill with seawater at high tide, then letting the water evaporate to leave the ionic compounds behind. The salt prepared this way is mostly sodium chloride, with a wide variety of other ions in smaller amounts (sulfate, magnesium, potassium, calcium, and many more). Sea salt is considered to be more of a delicacy when cooking as many chefs claim it tastes better. It is also more expensive to produce than normal table salt, and lacks the iodide that is added to normal table salt to prevent thyroid conditions caused by iodide deficiency.

Mixture Mass Percentages

In a similar way, a mixture of substances can also be characterized by the mass percentages of its components. For example, we might ask how much of seawater, by weight, does the salt account for? Experimentally, if we evaporate the water from one kilogram of seawater, we find that about 35 grams of salt are left behind. The mass percent of salt in seawater, then, is 3.5%. (Figure 6-6)

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Section 6: Chemical Reactions and Equations

In chemical reactions, scientists bring different types of molecules together. Some chemical bonds are broken, new chemical bonds are formed, and the result is a different set of molecules from the original reactants.

Chemical reactions can be represented on paper with equations. Unlike mathematical equations, which are built around an equals (=)sign, chemical equations show the changes in molecules when a chemical reaction occurs and are built around an arrow (→). For example:

$$CO_2 + H_2O \rightarrow H_2CO_3$$

For example, when carbon dioxide (CO_2) mixes with water (H_2O), these substances react to make carbonic acid (H_2CO_3). To the left of the arrow are the reactants, CO_2 and H_2O, i.e., the molecules we start out with. To the right is the product, H_2CO_3, the molecule we end up with. The reactants undergo changes in their bonds to produce the products.

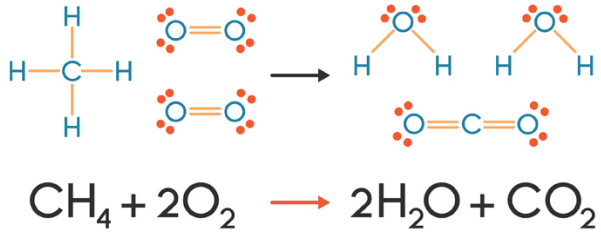

Figure 6-7. Writing Chemical Equations

Methane (CH_4) and dioxygen (O_2) react to make water (H_2O) and carbon dioxide (CO_2). The Lewis structure for each molecule is on top, and the molecular formula is on the bottom. One carbon atom, three oxygen atoms, and two hydrogen atoms yield one carbon atom, three oxygen atoms, and two hydrogen atoms.

Balanced Equations

When writing chemical equations, some rules must be followed. Note in our example of methane combustion (Figure 6-7) that on the left-hand side of the equation, there is one atom of carbon, four atoms of oxygen, and four atoms of hydrogen. Therefore, there must also be one carbon atom, four oxygen atoms, and four hydrogen atoms on the right-hand side of the equation. The reactants combine to make the products, with nothing left over and nothing missing. The reaction just reorganizes which atoms are bonded to others. (Remember Unit 1, in which French chemist Antoine Lavoisier demonstrated conservation of matter in the 1770s. "Nothing is created. Nothing is destroyed. Everything is transformed," Lavoisier famously stated.)

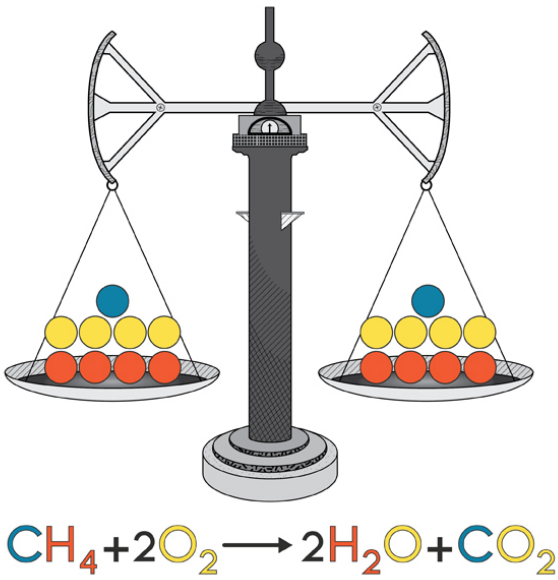

Figure 6-8. Reaction of Methane Combustion

In this combustion reaction, methane combines with oxygen to make water and carbon dioxide. Looking at an inventory of the atoms, note how the number of atoms of each type on each side of the equation match perfectly. This is because this equation is balanced. In order to balance this equation, it took two oxygen molecules and two water molecules, which is why both of those chemicals have coefficients of two in the balanced reaction.

This rule is always true for any properly written chemical equation, and we use the term "balanced" to describe such equations. A balanced equation has the same numbers of each type of atom on both sides of the equation. (Figure 6-8) In order for this equation to be written with formulas and be balanced, it has to have the number 2 appear before both the water and the dioxygen molecules. This number is called a **coefficient**, or a stoichiometric coefficient. Normally, when we see an equation, if there is no number written before a compound there is an implied 1 there, meaning that one of that compound is reacting. In the next section, we will see that these coefficients are very important for quantifying what's happening during a chemical reaction.

Similarly, while electrons are negatively charged and move around between atoms and molecules during the course of a reaction, electrons are neither created nor destroyed by a reaction. So, the numbers of electrons present at the beginning and end of a reaction must be the same, and thus the net charges (or total charges) must be equal on both sides of a balanced equation. For example, when solid lead sulfate (PbSO4)—the "lead" in a lead-acid car battery—is dissolved in water, it breaks down into its component ions. (Figure 6-9)

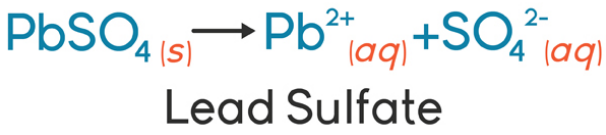

Figure 6-9. The Dissociation of Lead (II) Sulfate into Its Constituent Ions

The net charge (or total charge) must be equal on both sides of a balanced equation. The charge for lead sulfate on the left is zero. Looking at the products of the reaction, the 2+ and 2- charges for its constituent ions on the right added together also equal zero. Therefore, the charges are balanced.

Note that the little subscripts in parentheses in Figure 6-9 are used in chemical equations to indicate what phase the substance is in. The (*s*) on the $PbSO_4$ indicates that it is in solid form, while the (*aq*) subscript stands for "aqueous," and is attached to the ions that have been dissolved in water. We can also add subscripts of (*l*) for liquid phase chemicals and (*g*) for gas phase chemicals.

Glossary

Coefficient
In a balanced chemical equation, the number that appears before one of the compounds in the reaction. A pair of coefficients represent the ratio of one product or reactant in relation to the other reactants or products.

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Section 7: Stoichiometry

Now that we know that a balanced chemical reaction shows us where the atoms come from, and go to during the reaction, we want to find a way to use this inventory to help us figure out how much of these chemicals are present when we run reactions. Not every equation involves all chemicals with coefficients of ones in front of them. Sometimes things react with different coefficients or in different stoichiometric ratios. Stoichiometry is the branch of chemistry that deals with the relationships between the amounts of substances that are involved during a chemical reaction. Or, sometimes, the ratio in which molecules combine in a chemical equation is called the stoichiometry of the reaction (from the Greek *stoicheion*, meaning "element" and *metron*, meaning "measure").

Figure 6-10. Limewater

The image on the left shows the production of limewater by creating a supersaturated solution of calcium hydroxide. Limewater is an important ingredient in the preparation of corn tortillas. The image on the right is a lithograph of women making tortillas.

For example, if we combine calcium hydroxide ($Ca(OH)_2$) with carbonic acid (H_2CO_3), we get calcium carbonate ($CaCO_3$) and water. An aqueous solution of calcium hydroxide is called "limewater." Limewater has been used as an analytical test for the presence of carbon dioxide, because it turns a milky white as the insoluble calcium carbonate forms. This reaction is shown in Figure 6-10. Historically, limewater is important for making frescoes as well as preparing the corn for making traditional tortillas.

Finding the right numbers to put in front of the molecules is called "balancing the equation," and the numbers themselves are called "stoichiometric coefficients." We can think of them as the number of each type of reactant molecule that takes part in the reaction to produce the given numbers of product molecules. We can also think of the stoichiometric coefficients as the numbers of *moles* of the reactants producing the given numbers of moles of products. Thus, in the balanced reaction in Figure 6-11, one unit of calcium hydroxide ($Ca(OH)_2$) and one molecule of carbonic acid (H_2CO_3) react to produce one unit of calcium carbonate ($CaCO_3$) and two molecules of water. Similarly, two *moles* of calcium hydroxide will combine with one *mole* of carbonic acid to produce one *mole* of calcium carbonate and two *moles* of water.

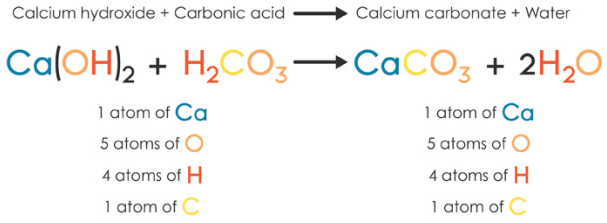


Figure 6-11. Exploring the Stoichiometry of a Balanced Equation

Because one molecule of calcium hydroxide is combining with the carbonic acid, and two molecules of water are being produced, we write the number two in front of the water to balance the equation. This means, in words, that one mole of calcium hydroxide reacts with one mole of carbonic acid to produce one mole of calcium carbonate and two moles of water.

With a balanced chemical reaction, anyone can now figure out exactly how much of a reactant that person would need for a reaction or how much of the product the reaction can be expected to make. It all comes down to the stoichiometric ratios between each of the substances in the balanced reaction. For example, if we want to know how much calcium hydroxide we need to react with four moles of carbonic acid, we can see that with a 1-to-1 ratio, we'd also need four moles of carbonic acid, and we'd expect to form four moles of calcium carbonate. Since we know the relationship between moles and masses (through molecular masses), we can easily convert these moles into masses that we can measure out using a scale or balance.

Unit 6: *Quantifying Chemical Reactions—Stoichiometry and Moles*

Section 8: Limiting Reagents

Figure 6-12. Making Chocolate Chip Cookies

This photo shows the exact amount of each ingredient needed to make exactly one full batch of chocolate chip cookies: brown sugar, flour, chocolate chips, butter, eggs, and a splash of vanilla. When we check to see if we have the ingredients to make a full batch of cookies, if any of the ingredients are lower than the called-for amount, we'd have to scale down the recipe to fit that ingredient: The ingredient that is less than is required for a full batch of cookies is a limiting ingredient. In chemistry, an ingredient that is used up first during a reaction is called the "limiting reagent."

The stoichiometric coefficients in a balanced chemical equation show the ratio in which the amounts of substances combine each time the reaction occurs. But, in an actual laboratory, we may not have exactly this ratio of molecules in our test tube or beaker. When this happens, one or more of the reactants will still be present even after all of the substances that can react with one another have reacted.

One can think of the chemical equation as a recipe for combining reactants to cook up one batch of the products. Imagine we were going to make a batch of 20 chocolate chip cookies (Figure 6-12) and had a recipe that called for:

- 2 cups of flour
- 1 cup of brown sugar
- 1 stick of butter
- 2 eggs
- 1 bag of chocolate chips
- 1 splash of vanilla

2 cups flour + 1 cup brown sugar + 1 stick of butter + 2 eggs + 1 bag of chocolate chips + 1 splash vanilla → 20 cookies

These quantities are the amounts required to make one batch of 20 cookies. If we went to the kitchen and found we had some of each of the ingredients, but only one cup of flour instead of two, we could still make cookies. But we couldn't make a whole batch. By cutting all the other ingredients in half, we can make a batch of 10 cookies. We could even consider the recipe in the form shown above like a balanced chemical reaction with stoichiometric coefficients in front of each ingredient. The amount of cookies we can make is limited by the amount of flour we have: We might say it is the "limiting ingredient."

If we also had only one-fourth of a stick of butter, then we could only make one-fourth of a batch of cookies, or only 5 cookies. Now, even though we still only have half as much flour as the recipe calls for, it doesn't matter because the butter is now our limiting ingredient: We will run out of butter before we run out of flour. Since we started with that cup of flour, if we used up all of the one-fourth stick of butter, it would use up half a cup of flour, leaving us with one cup of flour for baking again at a later time.

A similar situation exists when we combine molecules in the reaction described by a chemical equation. Returning to the chemical reaction for the combustion of methane we balanced in Section 6 (Figure 6-13):

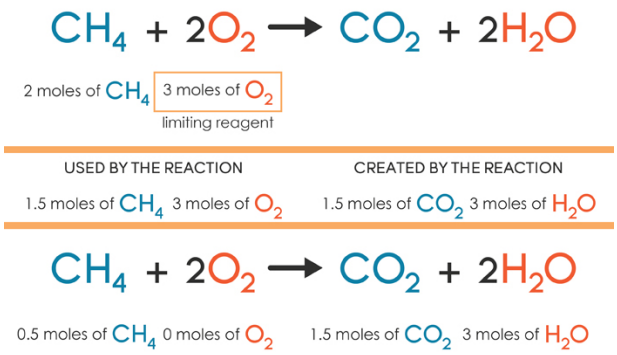


Figure 6-13. Recognizing Limiting Reagents

The top equation is a balanced equation showing the combustion of methane in the presence of oxygen. The first line shows the two starting reactants, and points out that the oxygen is the limiting reagent. Using the stoichiometric ratios along with the amount of oxygen present, the amount of substances used up and created by this reaction can be found. At the bottom of the figure, there is an inventory of what is left after the reaction is complete. Note that the only thing that is at zero is the limiting reagent that was completely used up.

Imagine that we have two moles of methane (CH_4) in a container, and we add enough air into the container so that there are three moles of oxygen (O_2). In this chemical reaction, each molecule of methane reacts with two molecules of oxygen. So, if we have two moles of methane, we need four moles of oxygen. Since we have provided only three moles of oxygen molecules, there are not enough to react with all of the methane. This makes the oxygen the limiting reagent. But some of the methane can still react, specifically one and a half moles of methane—until all three moles of oxygen are used up.

When we are done, we will have one and a half moles of carbon dioxide and three moles of water for products, as shown in the chemical equation. We will also have half of a mole of methane left over that just didn't react because there wasn't enough oxygen present. On the other hand, if we had mixed one mole of methane with three moles of oxygen, then the methane would have run out first and would have been the limiting reagent with some of the oxygen being left over.

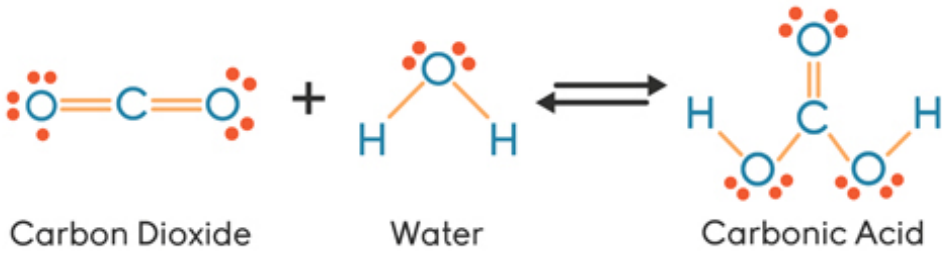
In actual laboratory work, when a reaction is carried out, it is unusual to have exactly the right ratio of the amounts of substances in the test tube. The reaction can continue to occur only until it runs out of the reactant molecule that there is the least of, relatively or stoichiometrically speaking. This reactant is referred to as the "limiting reagent" for that particular mixture of molecules. Ideally, manufacturers want their most expensive ingredient to be the limiting reagent for a production process—i.e., to have that ingredient run out first, so that they are not left with excess supplies of their most costly material because a cheaper reactant has been used up.

Unit 6: *Quantifying Chemical Reactions—Stoichiometry and Moles*

Section 9: Percent Yield

Equilibrium Reactions

In the reactions so far, we have drawn the arrow pointing from the reactants to the products. In reality, most chemical reactions can go either way. For example, water (H_2O) and carbon dioxide (CO_2) can react to produce carbonic acid (H_2CO_3). But it is also true that the carbonic acid can break down back into water and carbon dioxide. For a reaction that can go in both directions like this, we draw the arrow pointing in both directions in the chemical equation.



Looking at an Equilibrium Reaction. ©Science Media Group.

Note that even in a two-way reaction like this we still, by convention, refer to the molecules on the left as the "reactants" and those on the right as the "products," unless otherwise specified. We use the term "the forward direction of the reaction" to indicate the formation of products from reactants (shown by the arrow pointing to the right), and the term "the reverse direction of the reaction" to indicate the formation of reactants from products (shown by the arrow pointing to the left).

So, if the reaction can go in both directions, what happens if we put carbon dioxide and water together? Does anything happen? The answer is yes, the reaction proceeds to the right and carbonic acid is produced. But as soon as carbonic acid begins to accumulate, the reverse reaction begins to occur and the carbonic acid starts to break down. If we leave the reaction mixture alone for a long time, we'll find that the amounts of water, carbon dioxide, and carbonic acid eventually stop changing. While their total amounts are not changing, the reactions are still occurring so that products and reactants are still rapidly converting back and forth, but at rates that don't affect the totals. At this point there is carbonic acid, the product, in the mixture, so we must conclude that the reaction occurred to some extent. But not all of the reactants have disappeared, so we say the reaction has not "gone to completion." We call this an "equilibrium reaction."

So, how much product do we end up with in a chemical reaction? It turns out that some chemical reactions will never be 100% complete due to a variety of factors. In some cases, there are impurities in the reagents or other side reactions that take place unexpectedly with one of the reagents. And in some cases, there are reactions that reach equilibrium where they stop short of making 100% of the products. Unit 9 and the sidebar in this section will explore equilibrium reactions in more detail. To determine this, we need to figure

out the degree to which a reaction has gone to completion, which we describe with a quantity called the "**percent yield**." To calculate the percent yield of a reaction, we first determine the number of moles of product we would have if all of the limiting reagent were converted to products. This amount of product is called the **theoretical yield** of a reaction.

As an example, consider the reaction of carbon monoxide (CO) with hydrogen gas (H_2) to produce methane (CH_4) and water (H_2O). (Figure 6-14)

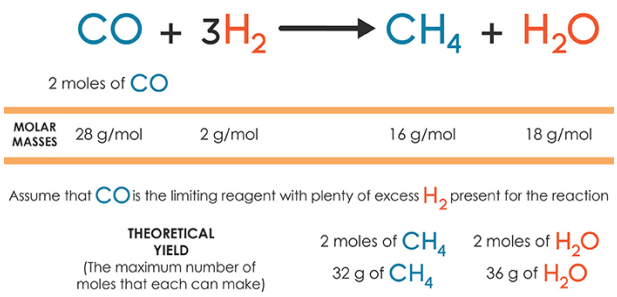


Figure 6-14. Finding the Theoretical Yield

To calculate the percent yield of a reaction, we determine the number of moles of product we would have if every molecule of the limiting reagent were converted to products; we call this the "theoretical yield." In this example, we are assuming that we have two moles (or 56 grams) of carbon monoxide with an unlimited amount of hydrogen gas. Therefore, the carbon monoxide is our limiting reagent and that's the amount in moles we will use to stoichiometrically determine the maximum amount of each product we can make. Thus, we can make two moles of either one of the two products because all the ratios are 1-to-1. When the reaction is done in the laboratory, we measure the actual yield and compare it to the theoretical yield to find the percent yield.

If we mix 56 grams of carbon monoxide with a large excess of hydrogen, how much methane can we expect to see? First, note that carbon monoxide is the limiting reagent: The reaction equation shows each mole of carbon monoxide combining with three moles of hydrogen; since we are told we have an excess of hydrogen, we know that there must be more than six moles of it around to react completely with the carbon monoxide. If this happens, the reaction equation tells us that for every mole of carbon monoxide, we should get one mole of methane. Since methane weighs 16 g/mol, this would be 32 grams of methane, which is our theoretical yield.

But wait! Because nature is not perfect, we don't expect to see the reaction go to completion. Not necessarily all of the carbon monoxide will have reacted when we go to collect the products, so really we expect to find some smaller amount of methane produced.

When we are finished with a reaction in the laboratory, we can measure the amount of product that was actually isolated, and compare it to the theoretical yield. This is expressed as the percentage of the theoretical yield we actually obtained; this is the quantity mentioned earlier called the "percent yield." It doesn't matter how we measure the amount of the theoretical or actual yield so long as we measure them both in the same units. The two common ways of quantifying the amounts of the product formed are by

using moles or masses for the products. Both these methods can be seen in Table 6-2. For example, if we found that the reaction described above produced only 20 grams of methane (or 1.25 moles of methane), we would say we had a percent yield of 63%.

Table 6-2. Percent Yield

$$\text{Percent Yield} = \frac{\text{Actual Yield}}{\text{Theoretical Yield}} \times 100$$

Example:

$$\text{Percent Yield} = \frac{20 \text{ grams of } CH_4}{32 \text{ grams of } CH_4} \times 100 = 63\%$$

OR

$$\text{Percent Yield} = \frac{1.25 \text{ moles of } CH_4}{2 \text{ moles of } CH_4} \times 100 = 63\%$$

In general, we say that a reaction which shows 100% yield "went to completion," and a reaction with 0% yield did not occur at all. So, what does it mean when a reaction has a 50% yield? Well, that means that it didn't reach its theoretical maximum, and there are several main factors that contribute to that. For example, we usually talk about yields in terms of the isolated yield; this means we have collected our purified product in a new container. But just the process of running the experiment means we can spill some, some will be stuck to the sides of the container, and, in many cases, purifying a product to make sure it is only what we want causes some of the good product to be removed with the impurities. Combine that with some reactions having unwanted side reactions and others being equilibrium reactions that will never reach completion, and there are a lot of commonplace factors that keep yields of reactions far below 100%. And, in some cases, we were just impatient and collected the product before the reaction was complete because the reaction was slower than the time we had allotted.

Glossary

Percent yield

The degree to which a reaction has gone to completion.

Theoretical yield

The number of moles of product we would have if all of the limiting reagent were converted to products.

Unit 6: *Quantifying Chemical Reactions—Stoichiometry and Moles*

Section 10: Conclusion

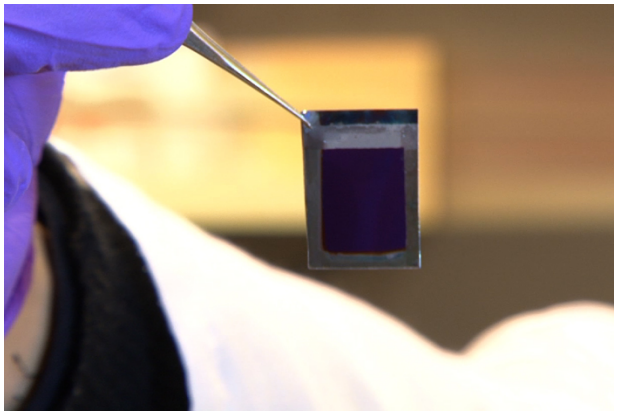


Figure 6-15. Artificial Leaf Using Light Energy to Split Water into Hydrogen and Oxygen Molecules

Professor Dan Nocera and his team at MIT are developing a technology in the lab that is similar to what happens in green plants: Energy from light is converted into chemical energy that can be stored as a fuel—in this case, hydrogen gas. The reaction can be written as $2H_2O \rightarrow 2H_2 + O_2$. This balanced chemical equation can be used to predict how many grams of hydrogen fuel will result from the conversion of any given amount of water.

Keeping track of the details is key to all scientific study. In chemistry, we take meticulous care to accurately describe what we have and what we may produce by using empirical formulas, molecular formulas, moles, and balanced chemical reactions. (Figure 6-15) Because we work with such incredibly small units (atoms and molecules), we have a lot of details to track. A convenient number of atoms or molecules to work with is a mole—meaning there are 6.02214×10^{23} atoms or molecules (Avogadro's number) of the thing in which we are interested. Chemists use moles in chemical equations to specify how much we start with (reactants), finish with (product), and have left over (yields, which may be affected by limiting reagents). All together, working with the amounts of substances as measured in moles, along with a balanced chemical reaction, encompasses the field of stoichiometry.

In Unit 7, we'll look at how we measure and deal with the other important quantity in chemical reactions, the energy.

Unit 6: *Quantifying Chemical Reactions—Stoichiometry and Moles*

Section 11: Further Reading

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