Chemical Formulas

To become familiar with chemical formulas and how they are obtained.

- balance
- 250-mL beaker
- Bunsen burner
- evaporating dish
- 50-mL graduated cylinder
- ring stand and ring
- stirring rod
- wire gauze

- crucible and cover
- clay triangle
- 6 M HCl
- granular zinc, about 1 g
- copper wire, about 2 g
- powdered sulfur, about 3 g
- carborundum boiling chips, or glass beads

Just as a secretary uses shorthand in order to take dictation at a greater speed, chemists use a shorthand notation of their own to indicate the exact chemical composition of compounds (chemical formulas). We then use these chemical formulas to indicate how new compounds are formed by chemical combinations of other compounds (chemical reactions). However, before we can learn how chemical formulas are written, we must first acquaint ourselves with the symbols used to denote the elements from which these compounds are formed.

Symbols and Formulas

We generally use two letters to symbolize a chemical element. These symbols are derived, as a rule, from the first two letters or first syllable of the elements name.

We can combine the symbols to denote the formulas for compounds in the following fashion. The formula CO (read “carbon monoxide”) means that one atom of carbon, C, combines with one of oxygen, O, to form the compound carbon monoxide. Similarly, in the compound CHCl₃, one atom of carbon, C, is combined with one atom of hydrogen, H, and three atoms of chlorine. The subscripts, 3 on the chlorine and 1 (understood) on both the carbon and hydrogen, imply exactly this. Thus, our chemical shorthand indicates the precise combining ratios of the chemical elements that form the molecule. Each and every molecule of carbon monoxide contains one atom of carbon and one of oxygen, just as each and every molecule of chloroform contains exactly one atom each of carbon and hydrogen and three of chlorine. Every chemical compound has this property; that is, every compound is composed of definite numbers of whole atoms in fixed proportions.
Atom Weights
It is important to know something about masses of atoms and molecules. We can measure the masses of individual atoms with a high degree of accuracy. We know, for example, the hydrogen-1 atom has a mass of $1.6735 \times 10^{-24}$ g and the oxygen-16 atom has a mass of $1.674 \times 10^{-24}$ g. Because it is cumbersome to express such small masses in grams we use a unit called the atomic mass unit, or amu. An amu equals $1.66054 \times 10^{-24}$ g. Most elements occur as mixtures of isotopes. The average atomic mass of each element expressed in amu is also known as its atomic weight. The atomic weights of the elements listed both in the table of elements and in the periodic table in Appendices C and D, respectively, are in amu.

Formula and Molecular Weights
The formula weight of a substance is merely the sum of atomic weights of each atom in its chemical formula. For example, HNO$_3$, nitric acid has a formula weight of 63.0 amu.

$$\text{FW} = (\text{AW of H}) + (\text{AW of N}) + 3(\text{AW of O})$$

$$= 1.0 \text{ amu} + 14.0 \text{ amu} + 3(16.0 \text{ amu})$$

$$= 63.0 \text{ amu}$$

If the chemical formula of a substance is its molecular formula, then the formula weight is also called the molecular weight. For example, the molecular formula for formaldehyde is CH$_2$O. The molecular weight of formaldehyde is therefore

$$\text{MW} = 12 \text{ amu} + 2(1.0 \text{ amu}) + 16.0 \text{ amu}$$

$$= 30.0 \text{ amu}$$

For ionic substances such as NaCl that exist as three dimensional arrays of ions, it is not appropriate to speak of molecules. Similarly, the terms molecular weight and molecular formula are inappropriate for these ionic substances. It is correct to speak of their formula weight, however. Thus, the formula weight of NaCl is:

$$\text{FW} = 23.0 \text{ amu} + 35.5 \text{ amu}$$

$$= 58.5 \text{ amu}$$

Percentage Composition From Formulas
New compounds are made in laboratories every day, and the formulas of these compounds must be determined. The compounds are often analyzed for their percentage composition (i.e., the percentage by mass of each element present in the compound). The percentage composition is useful information in establishing the formula for the substance. If the formula of a compound is known calculating the percentage composition is a straight-forward matter. In general, the percentage of an element in a compound is given by

$$\frac{(\text{Number of atoms of element})(\text{AW})}{\text{FW of compound}} \times 100$$
If we wanted to know the percentage composition of formaldehyde, CH₂O, whose formula weight is 30.0 amu we proceed as follows:

\[
\%C = \frac{12.0 \text{ amu}}{30.0 \text{ amu}} \times 100 = 40.0\%
\]

\[
\%H = \frac{2(1.0 \text{ amu})}{30.0 \text{ amu}} \times 100 = 6.7\%
\]

\[
\%O = \frac{16.0 \text{ amu}}{30.0 \text{ amu}} \times 100 = 53.3\%
\]

**The Mole**

Even the smallest samples we use in the laboratory contain an enormous number of atoms. A drop of water contains about \(2 \times 10^{21}\) water molecules! The unit that the chemist uses for dealing with such a large number of atoms, ions or molecules is the **mole**, abbreviated mol. Just as the unit dozen refers to 12 objects, the mole refers to a collection of \(6.02 \times 10^{23}\) objects. This number is called Avogadro's number. Thus, a mole of water molecules contains \(6.02 \times 10^{23}\) \(\text{H}_2\text{O}\) molecules and a mol of sodium contains \(6.02 \times 10^{23}\) \text{Na} atoms. The mass (in grams) of 1 mol of a substance is called its **molar mass**. The molar mass (in grams) of any substance is numerically equal to its formula weight. Thus:

One \(\text{CH}_2\text{O}\) molecule weighs 30.0 amu; 1 mol \(\text{CH}_2\text{O}\) weighs 30.0 g and contains \(6.02 \times 10^{23}\) \(\text{CH}_2\text{O}\) molecules.

One \text{Na} atom weighs 23.0 amu; 1 mol \text{Na} weighs 23.0 g and contains \(6.02 \times 10^{23}\) \text{Na} atoms.

It is a simple matter to calculate the number of moles of any substance whose weight we can obtain. For example, suppose we have one quart of rubbing alcohol (generally isopropyl alcohol) and know its density to be 0.785 g/mL and we want to know how many moles this is. First we need to convert the volume to our system of units. Since 1 qt is 0.946 L and 1 L contains 1000 mL, our quart of isopropyl alcohol is

\[
(1 \text{ qt})\left(\frac{0.946 \text{ L}}{1 \text{ qt}}\right)\left(\frac{1000 \text{ mL}}{1 \text{ L}}\right) = 946 \text{ mL}
\]

we can now calculate the weight:

\[
946 \text{ mL} \times 0.785 \text{ g/mL} = 743 \text{ g}
\]

We next need the chemical formula for isopropyl alcohol. This is \(\text{C}_3\text{H}_7\text{OH}\). The molecular weight is, therefore,

<table>
<thead>
<tr>
<th>Component</th>
<th>Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Weight carbon</td>
<td>(3 \times 12.0 = 36.0 \text{ amu})</td>
</tr>
<tr>
<td>Weight hydrogen</td>
<td>(8 \times 1.0 = 8.0 \text{ amu})</td>
</tr>
<tr>
<td>Weight oxygen</td>
<td>(1 \times 16.0 = 16.0 \text{ amu})</td>
</tr>
</tbody>
</table>

Molecular weight \(\text{C}_3\text{H}_7\text{OH} = 60.0 \text{ amu}\)
Hence,

$$\text{Moles of C}_3\text{H}_7\text{OH} = \frac{(743 \text{ g C}_3\text{H}_7\text{OH}) \left( \frac{1 \text{ mol C}_3\text{H}_7\text{OH}}{60.0 \text{ g C}_3\text{H}_7\text{OH}} \right)}{1} = 12.4 \text{ mol}$$

Thus our quart of rubbing alcohol contains 12.4 mol of isopropyl alcohol. It should now be apparent to you how much information is contained in a chemical formula. After you have some feeling for the nature of different chemical substances, you should be able to read the labels of many household items and know what the chemical contents are and why they are there. We have often heard the phrase “What’s in a name?” The answer to this question when the name is that of a chemical compound takes on considerable meaning as we gain familiarity with that compound. For example the simple name carbon dioxide tells us precisely

1. The elements present, carbon and oxygen;
2. The combining ratios of these elements, one atom of carbon for every two atoms of oxygen in each molecule of carbon dioxide;
3. The molecular weight;
4. And, after we learn some chemistry, that we are speaking of a colorless gas, heavier than air, which will not support combustion and which is lethal simply because it will not allow us to take in oxygen when there is a lot of it around. We will also learn that it can be solidified by compression to produce the familiar dry ice.

All of this dialogue is simply to illustrate that chemical formulas are tremendously important, and it behooves us in the very beginning to have a firm understanding of just exactly what they are. It should also be evident that we must have some way of determining them precisely if they do contain so much information.

**Derivation of Formulas**

Suppose you were working in a hospital laboratory today, and suppose further that this morning the emergency ward admitted a patient complaining of severe stomach cramps and labored respiration and that this patient died within minutes of being admitted. Relatives of the patient later told you that he may have ingested some rat poison. You therefore had his stomach pumped to verify this or simply to determine the cause of death. One of the more logical things to do would be to attempt to isolate the agent that caused death and perform chemical analyses on it. Let’s suppose that this was done, and the analyses showed that the isolated chemical compound contained, by weight, 60.0 percent potassium, 18.5 percent carbon, and 21.5 percent nitrogen. What is the chemical formula for this compound? One simple and direct way of making the necessary calculations is as follows.

Assume you had 100 g of the compound. This 100 g therefore would contain

\[(100 \text{ g})(0.600) = 60.0 \text{ g potassium}\]
\[(100 \text{ g})(0.185) = 18.5 \text{ g carbon}\]
\[(100 \text{ g})(0.215) = 21.5 \text{ g nitrogen}\]

Chemical formulas tell what elements are present and the ratio of the number of atoms of the constituent elements. Hence, the next step is to determine the number of moles of each element present:
Moles potassium = \( \frac{60.0 \text{ g K}}{39.0 \text{ g K/mol K}} = 1.54 \text{ mol K} \)

Moles carbon = \( \frac{18.5 \text{ g C}}{12.0 \text{ g C/mol C}} = 1.54 \text{ mol C} \)

Moles nitrogen = \( \frac{21.5 \text{ g N}}{14.0 \text{ g N/mol N}} = 1.54 \text{ mol N} \)

Hence the chemical formula is \( K_{1.54}C_{1.54}N_{1.54} \). But molecules are not formed from partial atoms; therefore, the above numbers must be changed to whole numbers. This is accomplished by division of all subscripts by the smallest subscript. In this case, they are all the same:

\[ K_{1.54/1.54}C_{1.54/1.54}N_{1.54/1.54} = KCN \]

The smallest whole-number mole ratio is 1:1:1. Since KCN is a common rat poison, we may justifiably conclude that the relatives’ suggestion of rat-poison ingestion as the probable cause of death is correct.

The above calculation has given us what is known as the empirical formula. There is another type of chemical formula the molecular formula. The distinction between these two is simply that the empirical formula represents the smallest whole-number ratio of the combining atoms in a chemical compound, whereas the molecular formula gives the actual number of atoms in a molecule. Recall, however, as we stated earlier, that not all compounds exist as discrete molecules. This is true for most ionic compounds, whereas most covalent compounds do exist as discrete molecules. The distinction between empirical and molecular formulas may be clarified by the following example.

A chemical compound was found by elemental analyses to contain 92.3 percent carbon and 7.7 percent hydrogen by weight and to have a molecular weight of 78. The empirical formula may be obtained just as in the previous example—that is, in 100 g of the compound there are 92.3 g C and 7.7 g H. Hence,

\[ \text{Moles C} = \frac{92.3 \text{ g C}}{12 \text{ g C/mol C}} = 7.7 \text{ mol C} \]

\[ \text{Moles H} = \frac{7.7 \text{ g H}}{1.0 \text{ g H/mol H}} = 7.7 \text{ mol H} \]

The empirical formula is then \( C_{7.7}H_{7.7} \), or \( CH \), whose formula weight is 12 + 1 = 13. But the molecular weight of the compound is 78. Therefore, there are 78/13 = 6 empirical-formula weights in the molecular weight. The molecular formula is then \( C_6H_6 \).

In this experiment you will determine the empirical formulas of two chemical compounds. One is copper sulfide, which you will prepare according to the following chemical reaction:

\[ xCu(s) + yS_2(s) \rightarrow Cu_xS_y(s) \]

The other is zinc chloride, which you will prepare according to the chemical reaction:

\[ xZn(s) + yHCl(aq) \rightarrow Zn_xCl_y(s) + \frac{y}{2}H_2(g) \]

The objective is to determine the combining ratios of the elements (that is, to determine \( x \) and \( y \)) and to balance the chemical equations given above.
**PROCEDURE**

### A. Zinc Chloride

**CAUTION:** Zinc chloride is caustic and must be handled carefully in order to avoid any contact with your skin. Should you come in contact with it, immediately wash the area with copious amounts of water. Clean and dry your evaporating dish and place it on the wire gauze resting on the iron ring. Heat the dish with your Bunsen burner, gently at first, and then more strongly, until all of the condensed moisture has been driven off. This should require heating for about 5 min. Allow the dish to cool to room temperature on a heat-resistant pad (do not place the hot dish on the counter top) and weigh it. Record the weight of the empty evaporating dish.

Obtain a sample of granular zinc from your laboratory instructor and add about 0.5 g of it to the weighed evaporating dish. Weigh the evaporating dish containing the zinc and record the total weight. Calculate the weight of the zinc.

Slowly, and with constant stirring, add 15 mL of 6 M HCl to the evaporating dish containing the zinc. A vigorous reaction will ensue, and hydrogen gas will be produced. **NO FLAMES ARE PERMITTED IN THE LABORATORY WHILE THIS REACTION IS TAKING PLACE, SINCE WET HYDROGEN GAS IS VERY EXPLOSIVE.** If any undissolved zinc remains after the reaction ceases, add an additional 5 mL of acid. Continue to add 5-mL portions of acid as needed until all the zinc has dissolved.

Set up a steam bath as illustrated in Figure 5.1 using a 250-mL beaker, and place the evaporating dish on the steam bath. Heat the evaporating dish very carefully on the steam bath until most of the liquid has disappeared. Then remove the steam bath and heat the dish on the wire gauze. During this last stage of heating, the flame must be carefully controlled or there will be spattering, and some loss of product will occur. **DO NOT HEAT TO THE POINT THAT THE COMPOUND MELTS, OR SOME WILL BE LOST DUE TO SUBLIMATION.** Leave the compound looking somewhat pasty while hot.

Allow the dish to cool to room temperature and weigh it. Record the weight. After this first weighing, heat the dish again very gently; cool it and reweigh it. If these weighings do not agree within 0.02 g, repeat the heating.
and weighing until two successive weighings agree. This is known as drying to constant weight and is the only way to be certain that all the moisture is driven off. Zinc chloride is very deliquescent and so should be weighed quickly.

Calculate the weight of zinc chloride. The difference in weight between the zinc and zinc chloride is the weight of chlorine. Calculate the weight of chlorine in zinc chloride. From this information you can readily calculate the empirical formula for zinc chloride and balance the chemical equation for its formation. Perform these operations on the report sheet.

**B. Copper Sulfide**

Support a clean, dry porcelain crucible and cover on a clay triangle and dry by heating to a dull red in a Bunsen flame, as illustrated in Figure 5.2. Allow the crucible and cover to cool to room temperature and weigh them. Record the weight.

Place 1.5-2.0 g of tightly wound copper wire or copper turnings in the crucible and weigh the copper, crucible, and lid. Calculate the weight of copper. Record your results.

In the hood, add sufficient sulfur to cover the copper, place the crucible with cover in place on the triangle, and heat the crucible gently until sulfur ceases to burn (blue flame) at the end of the cover. Do not remove the cover while the crucible is hot. Finally, heat the crucible to dull redness for about 5 min.

Allow the crucible to cool to room temperature. This will take about 10 min. Then weigh with the cover in place. Record the weight. Again cover the contents of the crucible with sulfur and repeat the heating procedure. Allow the crucible to cool and reweigh it. Record the weight. If the last two
Experiment 5 • Chemical Formulas

Weightings do not agree to within 0.02 g, the chemical reaction between the copper and sulfur is incomplete. If this is found to be the case, add more sulfur and repeat the heating and weighing until a constant weight is obtained.

Calculate the weight of copper sulfide obtained. The difference in weight between the copper sulfide and copper is the weight of sulfur in copper sulfide. Calculate this weight. From this information the empirical formula for copper sulfide can be obtained, and the chemical equation for its production can be balanced. Perform these operations on your report sheet.

REVIEW QUESTIONS

Before beginning this experiment in the laboratory, you should be able to answer the following questions:

1. Define the term “compound”.
2. Why are atomic weights relative weights?
3. How do formula weights and molecular weights differ?
4. What is the percentage composition of CaCO3?
5. A substance was found by analysis to contain 65.95 percent barium and 34.05 percent chlorine. What is the empirical formula for the substance?
6. What is the law of definite proportions?
7. How do empirical and molecular formulas differ?
8. What is the weight in grams of one copper atom?
9. Soda-lime glass is prepared by fusing sodium carbonate, Na2CO3, limestone, CaCO3, and sand, SiO2. The composition of the glass varies, but the commonly accepted reaction for its formation is

   \[ \text{Na}_2\text{CO}_3(s) + \text{CaCO}_3(s) + 6\text{SiO}_2(s) \rightarrow \text{Na}_2\text{CaSi}_6\text{O}_{14}(s) + 2\text{CO}_2(g) \]

   Using this equation, how many kilograms of sand would be required to produce enough glass to make five thousand 400-g wine bottles?

10. Caffeine, a stimulant found in coffee and tea contains 49.5 percent C, 5.15 percent H, 28.9 percent N, and 16.5 percent O by mass. What is the empirical formula of caffeine? If its molar mass is about 195 g, what is its molecular formula?

11. An analysis of an oxide of nitrogen with a molecular weight of 92.02 amu gave 69.57 percent oxygen and 30.43 percent nitrogen. What are the empirical and molecular formulas for this nitrogen oxide? Complete and balance the equation for its formation from the elements nitrogen and oxygen.

12. How many lithium atoms are present in 0.01456 g of lithium?
A. Zinc Chloride

1. Weight of evaporating dish and zinc
2. Weight of evaporating dish
3. Weight of zinc

4. Weight of evaporating dish and zinc chloride:
   - first weighing
   - second weighing
   - third weighing

5. Weight of zinc chloride

6. Weight of chlorine in zinc chloride

7. Empirical formula for zinc chloride (show calculations)

8. Balanced chemical equation for the formation of zinc chloride from zinc and HCl

B. Copper Sulfide

1. Weight of crucible, cover, and copper
2. Weight of crucible and cover
3. Weight of copper

4. Weight of crucible, cover, and copper sulfide:
   - first weighing
   - second weighing
   - third weighing

5. Weight of copper sulfide

6. Weight of sulfur in copper sulfide
7. Empirical formula for copper sulfide (show calculations)

8. Balanced chemical equation for the formation of copper sulfide from copper and sulfur

QUESTIONS

1. Can you determine the molecular formula of a substance from its percent composition?

2. Given that zinc chloride has a formula weight of 136.28, what is its formula?

3. Can you determine the atomic weights of zinc or copper by the methods used in this experiment? How? What additional information is necessary in order to do this?