The Molecular Formula of a Compound

6.3

Determining the identity of an unknown compound is important in all kinds of research. It can even be used to solve crimes. **Forensic scientists** specialize in analyzing evidence for criminal and legal cases. To understand why forensic scientists might need to find out the molecular formula of a compound, consider the following example.

Suppose that a suspect in a theft investigation is a researcher in a biology laboratory. The suspect frequently works with formaldehyde, CH_2O. Police officers find traces of a substance at the crime scene, and send samples to the Centre for Forensic Science. The forensic analysts find that the substance contains a compound that has an empirical formula of CH_2O. Will this evidence help to convict the suspect? Not necessarily.

As you can see from Table 6.3, there are many compounds that have the empirical formula CH_2O. The substance might be formaldehyde, but it could also be lactic acid (found in milk) or acetic acid (found in vinegar). Neither lactic acid nor acetic acid connect the theft to the suspect. Further information is required to prove that the substance is formaldehyde. Analyzing the physical properties of the substance would help to discover whether it is formaldehyde. Another important piece of information is the molar mass of the substance. Continue reading to find out why.

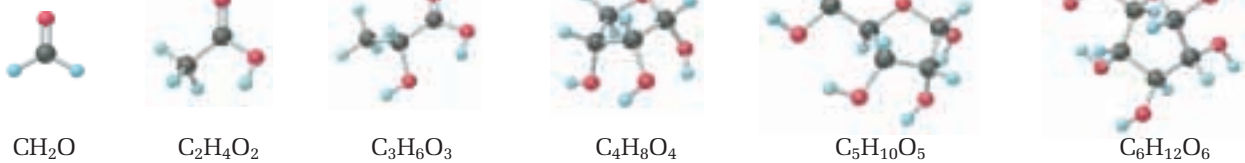
Section Preview/ Specific Expectations

In this section, you will

- **determine** the molecular formula of a compound, given the empirical formula of the compound and some additional information
- **identify** real-life situations in which the analysis of unknown substances is important
- **communicate** your understanding of the following terms: *forensic scientists*

Table 6.3 Six Compounds with the Empirical Formula CH_2O

Name	Molecular formula	Whole-number multiple	M (g/mol)	Use or function
formaldehyde	CH_2O	1	30.03	disinfectant; biological preservative
acetic acid	$C_2H_4O_2$	2	60.05	acetate polymers; vinegar (5% solution)
lactic acid	$C_3H_6O_3$	3	90.08	causes milk to sour; forms in muscles during exercise
erythrose	$C_4H_8O_4$	4	120.10	forms during sugar metabolism
ribose	$C_5H_{10}O_5$	5	150.13	component of many nucleic acids and vitamin B_2
glucose	$C_6H_{12}O_6$	6	180.16	major nutrient for energy in cells



CH_2O $C_2H_4O_2$ $C_3H_6O_3$ $C_4H_8O_4$ $C_5H_{10}O_5$ $C_6H_{12}O_6$

Determining a Molecular Formula

Recall the equation

Molecular formula subscripts = $n \times$ Empirical formula subscripts,
where $n = 1, 2, 3...$

Additional information is required to obtain the molecular formula of a compound, given its empirical formula. We can use the molar mass and build on the above equation, as follows:

Molar mass of compound = $n \times$ Molar mass of empirical formula,
where $n = 1, 2, 3...$

Careers in Chemistry

Analytical Chemistry

Ben Johnson, Steve Vezina, Eric Lamaze—all of these athletes tested positive for performance-enhancing substances that are banned by the International Olympic Committee (IOC). Who conducts the tests for these substances? Meet Dr. Christiane Ayotte, head of Canada's Doping Control Laboratory since 1991.

The Doping Control Lab

What happens to a urine sample after it arrives at the doping control lab? Technicians and scientists must be careful to ensure careful handling of the sample. Portions of the sample are taken for six different analytical procedures. More than 150 substances are banned by the IOC. These substances are grouped according to their physical and chemical properties. There are two main steps for analyzing a sample:

1. purification, which involves steps such as filtration and extraction using solvents, and
2. analysis by either gas chromatography, mass spectrometry, or high-performance liquid chromatography. Chromatography refers to certain methods by which chemists separate mixtures into pure substances.

For most substances, just their presence in a urine sample means a positive result. Other substances must be present in an amount higher than a certain threshold. According to Dr. Ayotte, a male athlete would have to consume "10 very strong French coffees within 15 min" to go over the 12 mg/L limit for caffeine. Ephedrines and pseudoephedrines, two decongestants that are found in cough remedies and that act as stimulants, have a cut-off level. This allows athletes to take them up to one or two days before a competition.

Challenges

Dr. Ayotte and her team face many challenges. They look for reliable tests for natural substances, develop new analytical techniques, and determine the normal levels of banned substances for male and female athletes. Dr. Ayotte must defend her tests in hearings and with the press, especially when high-profile athletes get positive results. Her dreams include an independent international doping control agency and better drug-risk education for athletes.

For Dr. Ayotte, integrity and a logical mind are essential aspects of being a good scientist.

Make Career Connections

1. For information about careers in analytical chemistry, contact university and college chemistry departments.
2. For information about doping control and the movement for drug-free sport, contact the Canadian Centre for Ethics in Sport (CCES), the World Anti-Doping Agency (WADA), and the Centre for Sport and Law.

Thus, the molar mass of a compound is a whole number multiple of the "molar mass" of the empirical formula.

Chemists can use a mass spectrometer to determine the molar mass of a compound. They can use the molar mass, along with the "molar mass" of a known empirical formula, to determine the compound's molecular formula. For example, the empirical formula CH has a "molar mass" of 13 g/mol. We know, however, that acetylene, C_2H_2, and benzene, C_6H_6, both have the empirical formula CH. Suppose it is determined, through mass spectrometry,

that a sample has a molar mass of 78 g/mol. We know that the compound is C_6H_6, since 6×13 g = 78 g, as shown in Table 6.4.

Examine the Sample Problem and Practice Problems that follow to learn how to find the molecular formula of a compound using the empirical formula and the molar mass of the compound.

Table 6.4 Relating Molecular and Empirical Formulas

Formula	Molar Mass (g)	Ratio
C_6H_6 molecular	78	$\frac{78}{13} = 6$
CH empirical	13	

Sample Problem

Determining a Molecular Formula

Problem

The empirical formula of ribose (a sugar) is CH_2O. In a separate experiment, using a mass spectrometer, the molar mass of ribose was determined to be 150 g/mol. What is the molecular formula of ribose?

What Is Required?

You need to find the molecular formula of ribose.

What Is Given?

You know the empirical formula and the molar mass of ribose.

Plan Your Strategy

Divide the molar mass of ribose by the "molar mass" of the empirical formula. The answer you get is the factor by which you multiply the empirical formula.

Act on Your Strategy

The "molar mass" of the empirical formula CH_2O, determined using the periodic table, is

$$12 \text{ g/mol} + 2(1) \text{ g/mol} + 16 \text{ g/mol} = 30 \text{ g/mol}$$

The molar mass of ribose is 150 g/mol.

$$\frac{150 \cancel{\text{ g/mol}}}{30 \cancel{\text{ g/mol}}} = 5$$

$$\begin{aligned}\text{Molecular formula subscripts} &= 5 \times \text{Empirical formula subscripts} \\ &= C_{1\times5}H_{2\times5}O_{1\times5} \\ &= C_5H_{10}O_5\end{aligned}$$

Therefore, the molecular formula of ribose is $C_5H_{10}O_5$.

Check Your Solution

Work backward by calculating the molar mass of $C_5H_{10}O_5$.
$(5 \times 12.01 \text{ g/mol}) + (10 \times 1.01 \text{ g/mol}) + (5 \times 16.00 \text{ g/mol}) = 150 \text{ g/mol}$
The calculated molar mass matches the molar mass that is given in the problem. The answer is reasonable.

Continued ...

CHEM FACT

Three classifications of food are proteins, fats, and carbohydrates. Many carbohydrates have the empirical formula CH_2O. This empirical formula looks like a hydrate of carbon, hence the name "carbohydrate." Glucose, fructose, galactose, mannose, and sorbose all have the empirical formula CH_2O since they all have the same molecular formula, $C_6H_{12}O_6$. What makes these sugars different is the way in which their atoms are bonded to one another. In Chapter 13, you will learn more about different compounds with the same formulas.

Continued ...
FROM PAGE 217

Practice Problems

17. The empirical formula of butane, the fuel used in disposable lighters, is C_2H_5. In an experiment, the molar mass of butane was determined to be 58 g/mol. What is the molecular formula of butane?
18. Oxalic acid has the empirical formula CHO_2. Its molar mass is 90 g/mol. What is the molecular formula of oxalic acid?
19. The empirical formula of codeine is $C_{18}H_{21}NO_3$. If the molar mass of codeine is 299 g/mol, what is its molecular formula?
20. A compound's molar mass is 240.28 g/mol. Its percentage composition is 75.0% carbon, 5.05% hydrogen, and 20.0% oxygen. What is the compound's molecular formula?

CHEM FACT

Codeine is a potent pain reliever. It acts on the pain centre in the brain, rather than interrupting pain messages from, for example, a headache or a sore arm. It is potentially habit-forming and classified as a narcotic.

Section Wrap-up

How do chemists obtain the data they use to identify compounds? In Investigation 6-A, you explored one technique for finding the percentage composition, and hence the empirical formula, of a compound containing magnesium and oxygen. In section 6.4, you will learn about another technique that chemists use to determine the empirical formula of compounds containing carbon and hydrogen. You will learn how chemists combine this technique with mass spectrometry to determine the compound's molecular formula. You will also learn about a new type of compound and perform an experiment to determine the molecular formula of one of these compounds.

Section Review

Unit Investigation Prep

Before you design your experiment to find the composition of a mixture, think about the relationships between different compounds. Suppose you have 5.0 g of copper. This copper reacts to form copper(II) chloride, also containing 5.0 g of copper. How can you determine the mass of copper(II) chloride formed?

1. K/U Explain the role that a mass spectrometer plays in determining the molecular formula of an unknown compound.
2. I Tartaric acid, also known as cream of tartar, is used in baking. Its empirical formula is $C_2H_3O_3$. If 1.00 mol of tartaric acid contains 3.61×10^{24} oxygen atoms, what is the molecular formula of tartaric acid?
3. MC Why is the molecular formula of a compound much more useful to a forensic scientist than the empirical formula of the compound?
4. K/U Vinyl acetate, $C_4H_6O_2$, is an important industrial chemical. It is used to make some of the polymers in products such as adhesives, paints, computer discs, and plastic films.
   (a) What is the empirical formula of vinyl acetate?
   (b) How does the molar mass of vinyl acetate compare with the molar mass of its empirical formula?
5. I A compound has the formula $C_{6x}H_{5x}O_x$, where x is a whole number. Its molar mass is 186 g/mol; what is its molecular formula?