6.9 Molecular Formulas

How clean is the air in your home? Despite the best air-filtering technology available, indoor air pollution is unavoidable. Some outdoor pollutants follow you in as you enter your home. However, most indoor pollutants come from one of two sources. They are either produced by chemical processes in the home, such as home heating, or released—"off-gassed"—by products that we bring into the home. A newly installed synthetic carpet, for example, releases a cocktail of volatile organic compounds (VOCs) into the air (**Figure 1**). You will learn more about indoor air pollutants in Section 11.5.

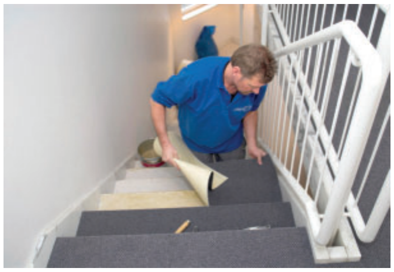


Figure 1 When new synthetic carpeting is installed, allow the area to air out for quite some time. This permits VOCs from the carpet and adhesives to escape.

You might recall that organic compounds consist mostly of carbon and hydrogen. VOCs are compounds that readily become gases at room temperature. VOCs can be natural or synthetic. For example, ethyl ethanoate is a VOC used in some nail polish removers and glues. It has relatively low toxicity and also occurs naturally in wine. Other VOCs, such as methylbenzene (toluene), are more toxic. Methylbenzene is a solvent used in glues and some flooring products. Toxic VOCs need to be handled with care to minimize exposure.

You may know someone who has allergies to "something in the air." The detection of indoor air pollutants is important in identifying possible causes of allergies. Fortunately, recent advances in analytical chemistry have made the detection of trace amounts of compounds in air possible. Scientists often use mass spectroscopy to detect and identify compounds in indoor air. As you learned in Section 6.8, a mass spectrometer is an analytical device that identifies compounds based on their molecular mass and characteristic fragment pattern. For example, **Figure 2** shows the mass spectrum of a contaminant in indoor air. This readout indicates that the compound has a molecular mass of 88 u.

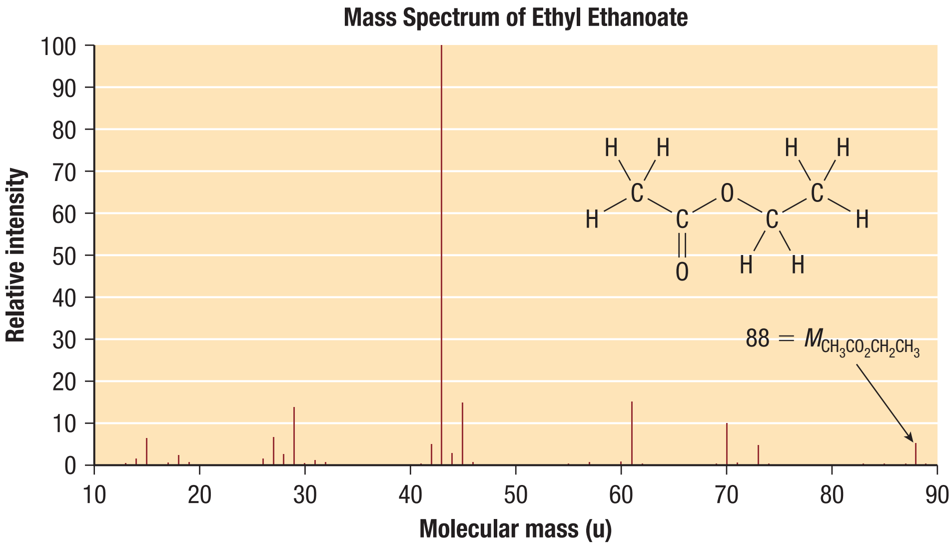
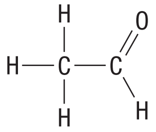
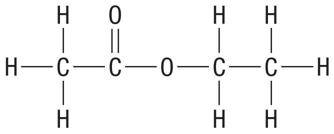
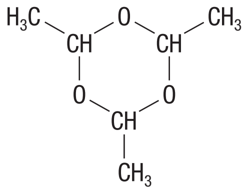


Figure 2 The largest molecular mass, 88 u, is the molecular mass of ethyl ethanoate. The other mass data are the masses of fragments of the molecule produced during the analysis. The molecular mass and fragment pattern together identify the compound.

The Importance of Molecular Formulas

Chemists use mass spectroscopy data together with an empirical formula to determine the molecular formula of a compound. Remember that the empirical formula gives only the simplest ratio of the atoms or ions of each element in the compound. The molecular formula, however, gives the exact number of atoms of each element present (Section 6.7). When we use the term "chemical formula" for a molecular compound, we are referring to the molecular formula. **Table 1** shows the molar mass and molecular formula of three organic compounds with the empirical formula C_2H_4O. However, only ethyl ethanoate has the molar mass 88.10 g/mol.

Table 1 Data for Identifying Three Organic Compounds with the Empirical Formula C_2H_4O

Compound	Molar mass (g/mol)	Molecular formula	Structural formula
ethanal (acetaldehyde) • used in the production of particle board	44.05	C_2H_4O	
ethyl ethanoate (ethyl acetate) • a solvent in glue	88.10	$C_4H_8O_2$	
2, 4, 6-trimethyl-1,3,5-trioxane (paraldehyde) • a central nervous system depressant, once used as an anesthetic	132.15	$C_6H_{12}O_3$	

Note that the molar masses of ethyl ethanoate and paraldehyde are whole-number multiples of the molecular mass of the empirical formula C_2H_4O. That explains why the subscripts in their molecular formulas are also multiples of the subscripts in C_2H_4O. For example, since 3(44.05 u) = 132.15 u, the molecular formula of paraldehyde must be $C_{2\times3}H_{4\times3}O_{1\times3}$, which equals $C_6H_{12}O_3$.

Mini **Investigation**

Comparing Molecules and Molecular Formulas

Skills: Predicting, Performing, Observing, Analyzing, Communicating — SKILLS HANDBOOK A2.4

In this activity you will construct molecules with the same empirical formula but different molecular formulas.

Equipment and Materials: molecular model kit

1. Construct 3 molecules of methanal (formaldehyde), CH_2O. Close the model kit box. For the rest of the activity, you will use only the atoms in these 3 molecules.
2. Take apart the methanal molecules and use some of the atoms to construct a molecule of a compound that has the molecular formula $C_2H_4O_2$. Note the number of starting atoms that are left over. Record the structural formula for this compound.
3. Using exactly the same atoms, construct a different molecule with the same molecular formula: $C_2H_4O_2$. Record the structural formula for this compound.
4. Construct a molecule with the molecular formula $C_3H_6O_3$. Record the structural formula for this compound.
5. Rearrange the atoms from Step 4 to form a different molecule. Record the structural formula for this compound.

A. What is the molecular mass of one molecule of methanal? T/I

B. How is the molar mass of methanal similar to its molecular mass and yet quite different? K/U

C. Predict the molecular mass of each molecule that you made in Steps 2, 3, 4, and 5. Comment on your predictions. T/I

D. Explain how the molecular masses of $C_2H_4O_2$ and $C_3H_6O_3$ can be predicted from the molecular mass of methanal. T/I

E. Why is determining the molecular formula of a compound an inadequate method of identifying the compound? Suggest a better way of identifying the compound. T/I

Investigation 6.9.1

Determining the Formula of a Hydrate (p. 304)
You will determine the formula of a sample of hydrated copper(II) sulfate by determining its percentage composition.

Determining Molecular Formulas

Chemists find that the molecular formula of a compound is far more useful than an empirical formula. This is because the molecular formula gives the exact composition of the compound, even though it does not always conclusively identify the compound. Determining the molecular formula from its empirical formula is an important step in analyzing an unknown compound.

Tutorial 1 Determining Molecular Formulas from Empirical Formulas

A compound's molar mass (based on the molecular formula) is always a whole-number multiple of the molar mass of the empirical formula. You can find this multiple, *x*, by dividing the molar mass of the compound by the molar mass of the empirical formula:

$$x = \frac{\text{molar mass of compound}}{\text{molar mass of empirical formula}}$$

You can then use this value to multiply the subscripts in the empirical formula to determine the subscripts in the molecular formula.

Sample Problem 1: Finding a Molecular Formula Given Its Empirical Formula

Determine the molecular formula of a compound with empirical formula CH_2 and molar mass 84.18 g/mol.

Given: empirical formula CH_2; molar mass of compound = 84.18 g/mol

Required: molecular formula of compound, C_xH_y

Solution:

Step 1. Find the empirical molar mass by adding the molar mass of each of the elements.

$$M_{CH_2} = 1\left(12.01\ \frac{g}{mol}\right) + 2\left(1.01\ \frac{g}{mol}\right)$$

$$M_{CH_2} = 14.03\ \frac{g}{mol}$$

Step 2. Solve for *x*, the mass multiple.

$$x = \frac{\text{molar mass of compound}}{\text{molar mass of empirical formula}}$$

$$= \frac{84.18\ \cancel{\frac{g}{mol}}}{14.03\ \cancel{\frac{g}{mol}}}$$

$$x = 6.000$$

Step 3. Therefore, the molar mass of the compound is 6 times the molar mass of the empirical formula. This means that the compound contains 6 times as many of each atom as given in the empirical formula. Multiplying each of the subscripts by 6 gives C_6H_{12}.

Statement: The molecular formula of the compound is C_6H_{12}.

Practice

SKILLS HANDBOOK A6.3, A6.5

1. Determine the molecular formulas given the following empirical formulas and molar masses: T/I
   (a) HO; 34.02 g/mol [ans: H_2O_2]
   (b) SO_2; 64.06 g/mol [ans: SO_2]
   (c) KSO_4; 270.32 g/mol [ans: $K_2S_2O_8$]
   (d) $C_3H_5O_3$; 445.40 g/mol [ans: $C_{15}H_{25}O_{15}$]

USING PERCENTAGE COMPOSITION AND MOLAR MASS DATA

You can also calculate the molecular formula of a compound if you know its percentage composition and its molar mass.

Sample Problem 2: Using Percentage Composition Data

Determine the molecular formula of vitamin C (ascorbic acid). This compound contains 40.5 % carbon, 4.6 % hydrogen, and 54.5 % oxygen. Its molar mass is 176.14 g/mol.

Given: 40.5 % C; 4.6 % H; 54.5 % O; molar mass = 176.14 g/mol

Required: molecular formula of ascorbic acid, $C_xH_yO_z$

Solution: A 100.0 g sample of this compound contains 40.5 g C, 4.6 g H, 54.5 g O.

Step 1. Determine the amount of each element in a 100.0 g sample.

$$n_C = (40.5\ \cancel{g})\left(\frac{1\ \text{mol}}{12.01\ \cancel{g}}\right)$$

$$n_C = 3.3722\ \text{mol [extra digits carried]}$$

$$n_H = (4.6\ \cancel{g})\left(\frac{1\ \text{mol}}{1.01\ \cancel{g}}\right)$$

$$n_H = 4.5545\ \text{mol [extra digits carried]}$$

$$n_O = (54.5\ \cancel{g})\left(\frac{1\ \text{mol}}{16.00\ \cancel{g}}\right)$$

$$n_O = 3.4063\ \text{mol [extra digits carried]}$$

A 100 g sample contains 3.37 mol of carbon, 4.55 mol of hydrogen, and 3.41 mol of oxygen.

Step 2. To determine the simplest ratio, divide the amount of each element by the smallest amount.

$$\frac{n_C}{n_C} = \frac{\cancel{3.3722\ \text{mol}}}{\cancel{3.3722\ \text{mol}}} = 1$$

$$\frac{n_O}{n_C} = \frac{3.4063\ \cancel{\text{mol}}}{3.3722\ \cancel{\text{mol}}} = 1.01$$

$$\frac{n_H}{n_C} = \frac{4.5545\ \cancel{\text{mol}}}{3.3722\ \cancel{\text{mol}}} = 1.35$$

We assign both carbon and oxygen a value of 1 and hydrogen a value of 1.35.

Step 3. These calculations give an empirical formula of $C_1H_{1.35}O_1$. Multiplying the subscripts by 3 gives $C_3H_4O_3$. Therefore, the empirical formula of the compound is $C_3H_4O_3$.

Step 4. Determine the molar mass of $C_3H_4O_3$.

$$M_{C_3H_4O_3} = 3\left(12.01\ \text{g/mol}\right) + 4\left(1.01\ \text{g/mol}\right) + 3\left(16.00\ \text{g/mol}\right)$$

$$M_{C_3H_4O_3} = 88.07\ \text{g/mol}$$

Step 5. Solve for the mass multiple.

$$x = \frac{\text{molar mass of compound}}{\text{molar mass of empirical formula}}$$

$$= \frac{176.14\ \cancel{\text{g/mol}}}{88.07\ \cancel{\text{g/mol}}}$$

$$x = 2.000$$

Step 6. The molar mass of the compound is twice the molar mass of the empirical formula. Multiplying each of the subscripts by 2 gives $C_6H_8O_6$.

Statement: The molecular formula of the compound is $C_6H_8O_6$.

Practice

SKILLS HANDBOOK A6.3, A6.5

2. Determine the molecular formula of each compound from the data provided. T/I C
   (a) A hydrocarbon containing 85.6 % carbon and the remainder hydrogen has a molar mass of 42.09 g/mol. [ans: C_3H_6]
   (b) A compound is 43.6 % phosphorus and the remainder oxygen. Its molar mass is 283.88 g/mol. [ans: P_4O_{10}]
   (c) A compound that contains 64.3 % carbon, 7.2 % hydrogen, and the remainder oxygen has a molar mass of 168.21 g/mol. [ans: $C_9H_{12}O_3$]

6.9 Summary

- The molecular formula gives the actual composition of a compound.
- The molecular formula is a whole-number multiple of the empirical formula. The multiplier can be determined using the equation

$$x = \frac{\text{molar mass of compound}}{\text{molar mass of empirical formula}}$$

- The molecular formula can be calculated from either the empirical formula and molar mass or the percentage composition and molar mass.

6.9 Questions

1. "A compound's molar mass (based on its molecular formula) is always a whole-number multiple, x, of the molar mass of its empirical formula." To test this statement, select a compound from Table 1 on page 297 and compare the molar masses of its empirical and molecular formulas. T/I
2. Determine the molecular formula for compounds with the following empirical formulas and molar masses: T/I C
   (a) NO_2; 92.02 g/mol
   (b) CH_2; 84.18 g/mol
   (c) $C_2H_3O_3$; 225.15 g/mol
   (d) CFBrO; 253.82 g/mol
3. Under what condition is the molecular formula of a compound the same as its empirical formula? K/U
4. Explain how two compounds can have the same percentage composition but different molecular masses. K/U
5. Empirical or molecular formulas can be used to describe molecular compounds. Can these concepts be used to describe ionic concepts as well? Explain your answer. K/U
6. Determine the empirical and molecular formulas of caffeine. Its molar mass is 194.19 g/mol and its percentage composition is 49.48 % carbon, 5.15 % hydrogen, 28.87 % nitrogen, and 16.49 % oxygen. T/I C
7. A substance believed to be an anabolic steroid (used by some athletes to build muscle) is seized from a professional athlete and analyzed. Combustion analysis reveals that the compound is 80.0 % carbon, 9.41 % hydrogen, and 10.6 % oxygen. A mass spectrometer analysis shows that the compound has a molar mass of 300.48 g/mol. K/U T/I C
   (a) Determine the molecular formula of the compound.
   (b) The substance is believed to be dianabol, a common performance-enhancing steroid. Is this analysis data sufficient to accuse the athlete of using dianabol? Why or why not?
8. Carbohydrates are compounds of carbon, hydrogen, and oxygen in which the ratio of hydrogen atoms to oxygen atoms is 2:1. A certain carbohydrate is known to be 40.0 % carbon. Its molar mass is approximately 180 g/mol. Determine the carbohydrate's empirical formula and molecular formula. T/I C
9. The media often highlight stories of athletes taking performance-enhancing substances such as steroids (**Figure 3**). T/I A

Figure 3 What are the effects of taking steroids?

   (a) Research the similarities and differences between anabolic steroids and human steroids.
   (b) Research the downside of "bulking up."

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