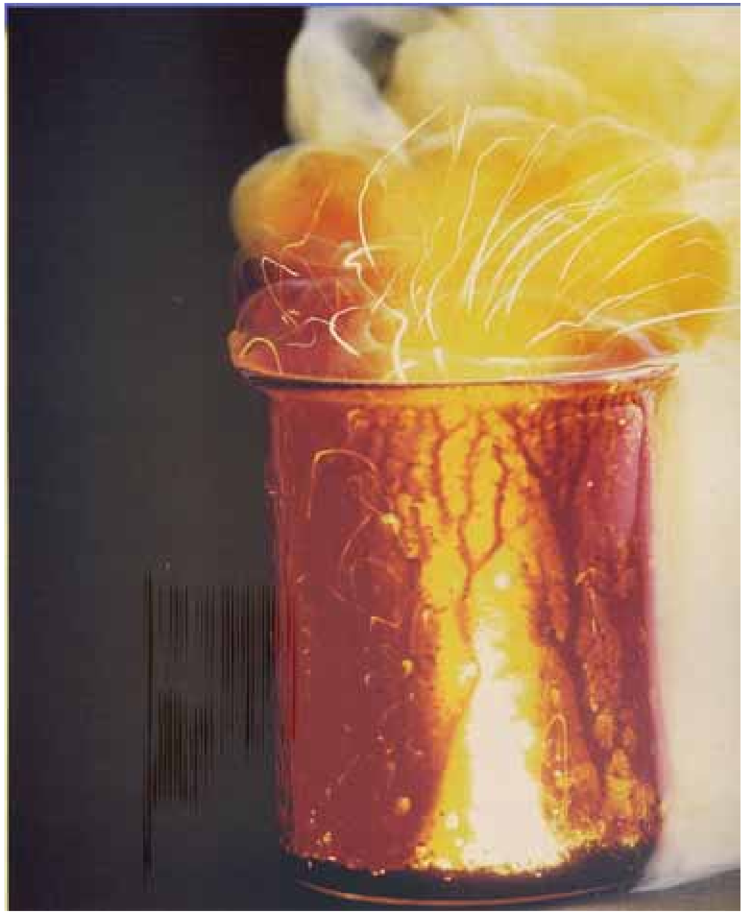
Chemistry

Zumdahl, 7th edition

歐亞書局

CH3 Stoichiometry



The violent chemical reaction of bromine and phosphorus.

Contents

Introduction

- Chemical reactions have a profound effect on our lives. There are many examples: Food is converted to energy in the human body; fuels and plastics are produced from petroleum; human insulin is produced in laboratories by bacteria;
- The central activity of chemistry is to understand chemical changes such as these, and the study of reactions occupies a central place in this book.

- chemical stoichiometry : the quantities of materials consumed and produced in chemical reactions.

3.1 Counting by Weighing

- In reality, jelly beans are not identical. For example, let's assume that you weigh 10 beans individually and get the following results:

Bean	**Mass**
1	5.1 g
2	5.2 g
3	5.0 g
4	4.8 g
5	4.9 g
6	5.0 g
7	5.0 g
8	5.1 g
9	4.9 g
10	5.0 g

Jelly beans can be counted by weighing.

- The *average mass* of the jelly beans.

$$\text{Average mass} = \frac{\text{total mass of beans}}{\text{number of beans}} = 5.0\ \text{g}$$

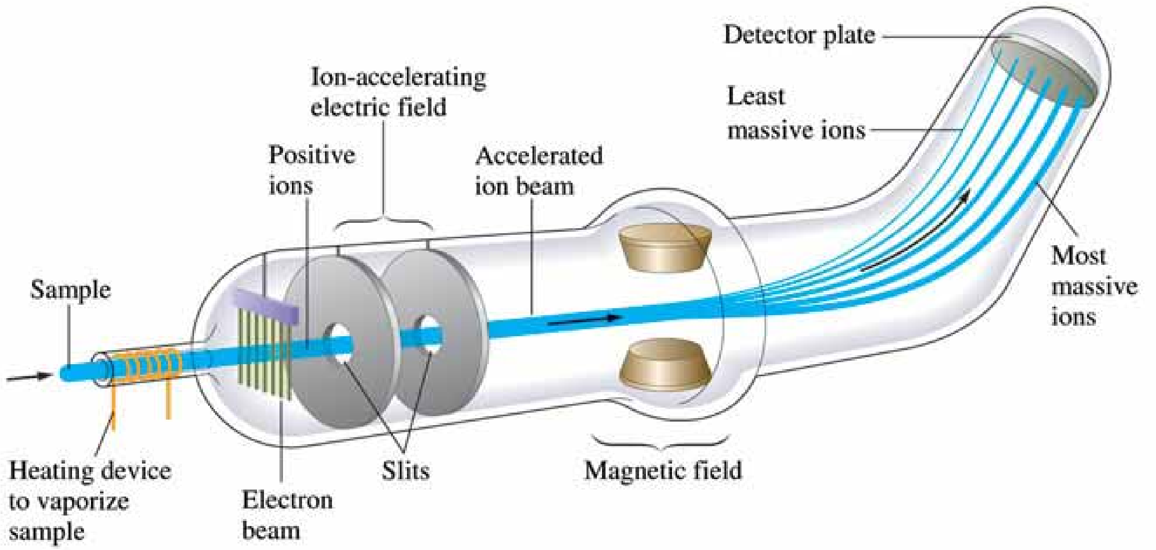
- For purposes of counting, the objects behave as though they were all identical, as though they each actually had the average mass.

3.2 Atomic Masses

- The first quantitative information about atomic masses came from the work of Dalton, Gay-Lussac, Lavoisier, Avogadro, and Berzelius.
- The modern system of atomic masses, instituted in 1961, is based on ^{12}C ("carbon twelve") as the standard. In this system, *^{12}C is assigned a mass of exactly 12 atomic mass units* (amu), and the masses of all other atoms are given relative to this standard.

- The most accurate method currently available for comparing the masses of atoms involves the use of the **mass spectrometer**.
- In this instrument, diagramed in Fig. 3.1, atoms or molecules are passed into a beam of high-speed electrons.

Figure 3.1



(left) A scientist injecting a sample into a mass spectrometer.
(above) Schematic diagram of a mass spectrometer.

- when ^{12}C and ^{13}C are analyzed in a mass spectrometer, the ratio of their masses is found to be

$$\frac{\text{Mass } ^{13}C}{\text{Mass } ^{12}C} = 1.0836129$$

- Since the atomic mass unit is defined such that the mass of ^{12}C is exactly 12 atomic mass units,

$$\text{Mass of } ^{13}C = (1.0836129)(\underset{\substack{\uparrow \\ \text{Exact number} \\ \text{by definition}}}{12 \text{ amu}}) = 13.003355 \text{ amu}$$

- The average atomic mass for carbon is computed as follows:

$$98.89\% \text{ of } 12 \text{ amu} + 1.11\% \text{ of } 13.0034 \text{ amu} =$$
$$(0.9889)(12 \text{ amu}) + (0.0111)(13.0034 \text{ amu}) = 12.01$$

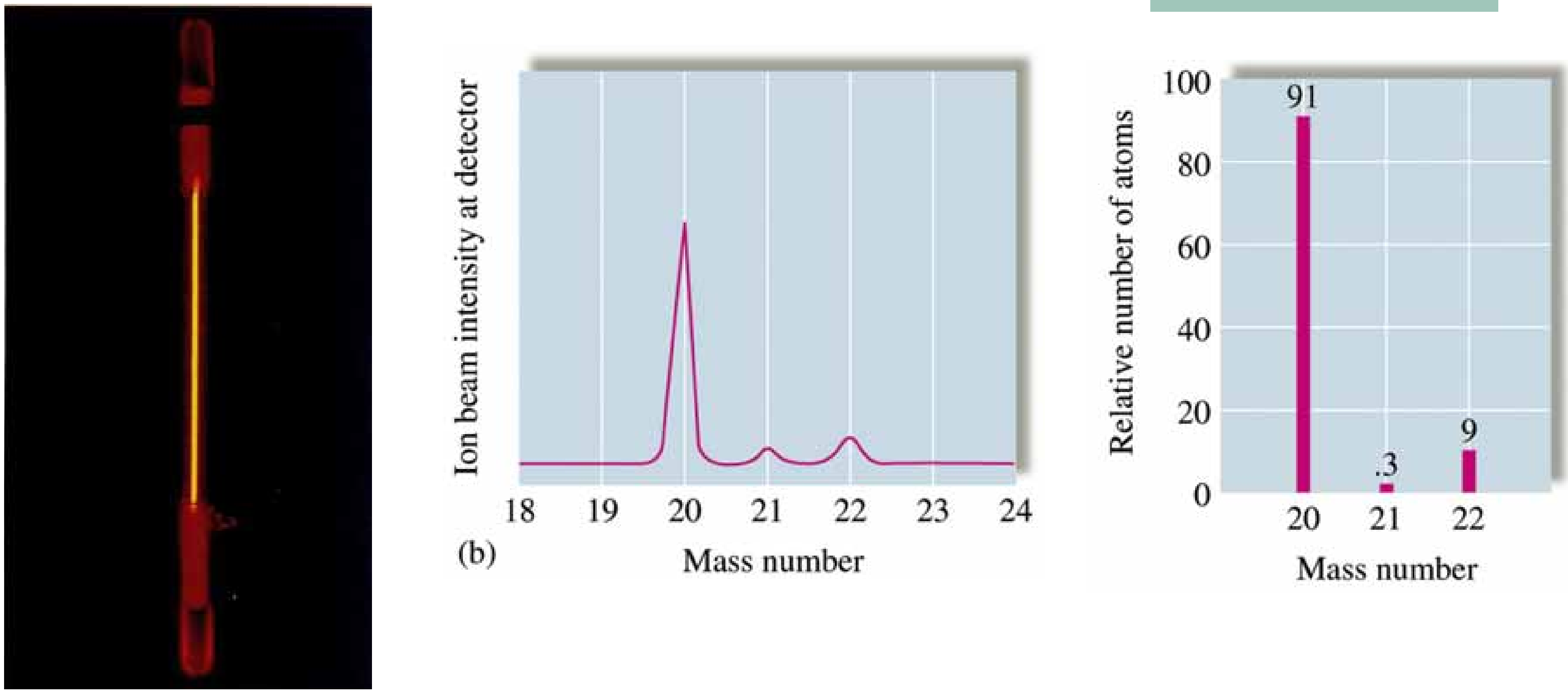
- In this text we will call the average mass for an element the **average atomic mass** or, simply, the *atomic mass* for that element.

- *Even though natural carbon does not contain a single atom with mass 12.01, for stoichiometric purposes, we can consider carbon to be composed of only one type of atom with a mass of 12.01.*

It is much easier to weigh out 600 hex nuts than count them one by one.

- When a sample of natural neon is injected into a mass spectrometer, the mass spectrum shown in Fig. 3.2 is obtained.
- The areas of the “peaks” or the heights of the bars indicate the relative abundances of $^{20}_{10}Ne$, $^{21}_{10}Ne$, and $^{22}_{10}Ne$ atoms.

Figure 3.2



Ion beam intensity at detector
18
19
20
21
22
23
24
(b)
Mass number
Relative number of atoms
100
80
60
40
20
0
91
.3
9
20
21
22
Mass number

Figure 3.2

(a) Neon gas glowing in a discharge tube. The relative intensities of the signals recorded when natural neon is injected into a mass spectrometer, represented in terms of (b) “peaks” and (c) a bar graph. The relative areas of the peaks are 0.9092 (^{20}Ne), 0.00257 (^{21}Ne), and 0.0882 (^{22}Ne); natural neon is therefore 90.92% ^{20}Ne, 0.257% ^{21}Ne, and 8.82% ^{22}Ne.

Sample Exercise 3.1 The Average Mass of an Element

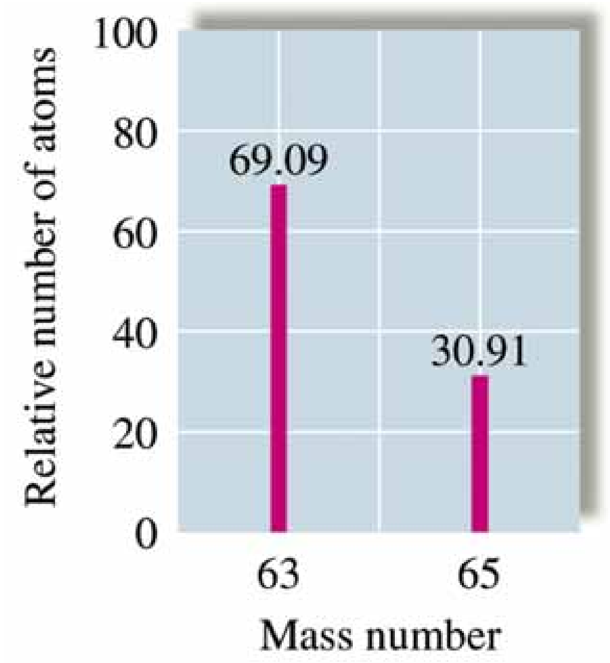
When a sample of natural copper is vaporized and injected into a mass spectrometer, the results shown in Fig. 3.3 are obtained. Use these data to compute the average mass of natural copper. (The mass values for ^{63}Cu and ^{65}Cu are 62.93 amu and 64.93 amu, respectively.)

Sample Exercise 3.1

Solution

The average mass of a copper atom is

$$\frac{6355 \text{ amu}}{100 \text{ atoms}} = 63.55 \text{ amu/atom}$$



Mass spectrum of natural copper.

See Exercises 3.27 and 3.28

3.3 The Mole

- **mole**: *the number equal to the number of carbon atoms in exactly 12 grams of pure ^{12}C.*
- Techniques such as mass spectrometry, which count atoms very precisely, have been used to determine this number as 6.02214×10^{23}.
- This number is called **Avogadro's number**.
- *One mole of something consists of 6.022×10^{23} units of that substance.*

- Since atoms are so tiny, a mole of atoms or molecules is a perfectly manageable quantity to use in a reaction (see Fig. 3.4).
- A sample of 12.01 grams of natural carbon contains the same number of atoms as 4.003 grams of natural helium. Both samples contain 1 mole of atoms (6.022×10^{23}).
- Table 3.1 gives more examples that illustrate this basic idea.

Figure 3.4

Proceeding clockwise from the top, samples containing one mole each of copper, aluminum, iron, sulfur, iodine, and (in the center) mercury.

TABLE 3.1 Comparison of 1 Mole Samples of Various Elements

Element	Number of Atoms Present	Mass of Sample (g)
Aluminum	6.022×10^{23}	26.98
Copper	6.022×10^{23}	63.55
Iron	6.022×10^{23}	55.85
Sulfur	6.022×10^{23}	32.07
Iodine	6.022×10^{23}	126.9
Mercury	6.022×10^{23}	200.6

- Thus the mole is defined such that a sample of a natural element with a mass equal to the element's atomic mass expressed in grams contains 1 mole of atoms.

$$6.022 \times 10^{23}\ \text{amu} = 1\ \text{g}$$

Exact number

- $1\ \text{amu} = 1.661 \times 10^{-24}\ \text{g}$
- This relationship can be used to derive the unit factor needed to convert between atomic mass units and grams.

Sample Exercise 3.2 Determining the Mass of a Sample of Atoms

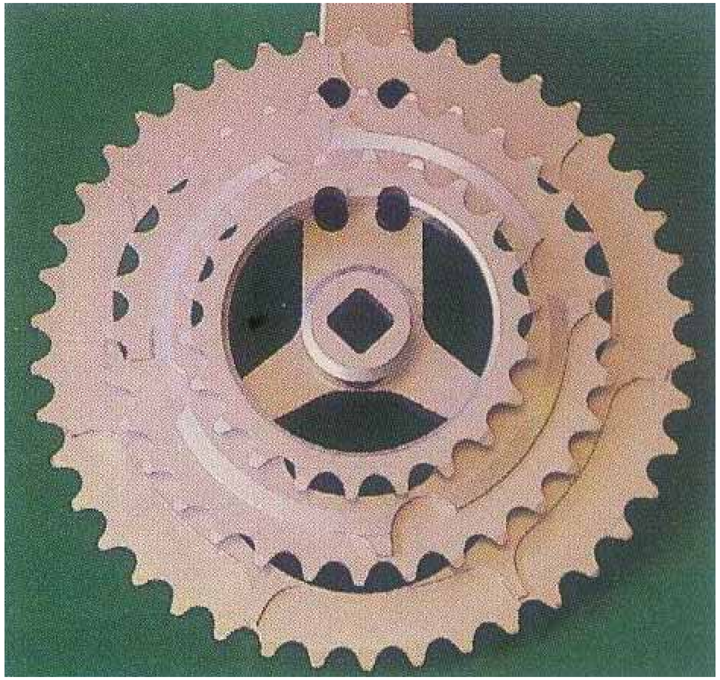
Americium is an element that does not occur naturally. It can be made in very small amounts in a device known as a particle accelerator. Compute the mass in grams of a sample of americium containing six atoms. (Am = 243)

Solution

The mass of six atoms is 1.46×10^3 amu. (243 x 6 =1458)
The mass of six americium atoms in grams is
2.42×10^{-21} g.

See Exercises 3.33

Sample Exercise 3.3 Determining Moles of Atoms



(left) Pure aluminum. (right) Aluminum alloys are used for many high-quality bicycle components, such as this chain wheel.

Sample Exercise 3.3

Compute both the number of moles of atoms and the number of atoms in a 10.0-g sample of aluminum.

Solution

The number of moles of aluminum atoms in 10.0 g is 0.371 mol Al atoms. (10.0/26.98 = 0.371 mol)

The number of atoms in 10.0 g (0.371 mol) of aluminum is 2.23×10^{23} atoms. ($0.371 \times 6.022 \times 10^{23} = 2.23 \times 10^{23}$ atoms)

See Exercises 3.34

Sample Exercise 3.5

Calculating the Number of Moles and Mass

Cobalt (Co) is a metal that is added to steel to improve its resistance to corrosion. Calculate both the number of moles in a sample of cobalt containing 5.00×10^{20} atoms and the mass of the sample.

Fragments of cobalt metal.

See Exercises 3.36

3.4 Molar Mass

- A chemical compound is a collection of atoms.
- The mass of 1 mole of methane can be found by summing the masses of carbon and hydrogen present:

Mass of 1 mole C	=	12.01 g
Mass of 4 mole H	=	$\underline{4 \times 1.008 \text{ g}}$
Mass of 1 mole CH4	=	16.04 g

- The **molar mass** of a substance is the mass in grams of one mole of the compound.

Sample Exercise 3.6

Calculating Molar Mass Ⅰ

Juglone (胡桃酮）, a dye known for centuries, is produced from the husks of black walnuts（黑胡桃樹）. It is also a natural herbicide (weed killer) that kills off competitive plants around the black walnut tree but does not affect grass and other noncompetitive plants. The formula for juglone is $C_{10}H_6O_3$. a. Calculate the molar mass of juglone.

b. A sample of 1.56×10^{-2} g of pure juglone was extracted from black walnut husks.
How many moles of juglone does this sample represent?

Sample Exercise 3.6

Solution

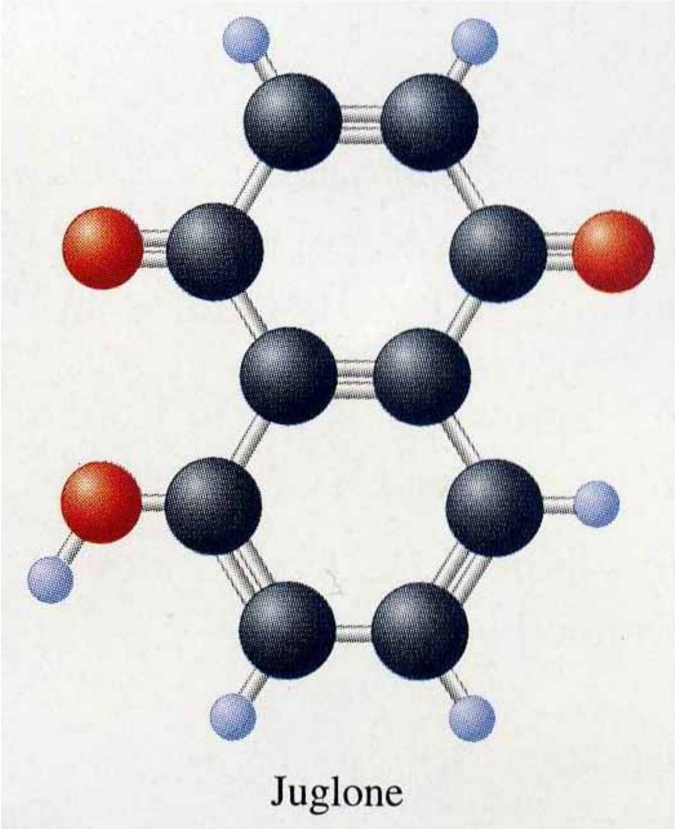
a.

10 C:	$10 \times 12.01\ g =$	$120.1\ g$
6 H:	$6 \times 1.008\ g =$	$6.048\ g$
3 O:	$3 \times 16.00\ g =$	$48.00\ g$
Mass of 1 mol $C_{10}H_6O_3$ =		$174.1\ g$

b.

1.56×10^{-2} g of pure juglone = 8.96×10^{-5} mol juglone

Sample Exercise 3.6



See Exercises 3.39 through 3.42

Sample Exercise 3.7 Calculating Molar Mass II

Calcium carbonate ($CaCO_3$), also called calcite, is the principal mineral found in limestone, marble, chalk, pearls, and shells of marine animals such as clams.

a. Calculate the molar mass of calcium carbonate.

b. A certain sample of calcium carbonate contains 4.86 moles. What is the mass in grams of this sample? What is the mass of the CO_3^{2-} ions present?

Sample Exercise 3.7

Solution

a.

1 Ca^{2+}:	1×40.08 g =	40.08 g
1 CO_3^{2-}:		
1 C:	1×12.01 g =	12.01 g
3 O:	3×16.00 g =	48.00 g
Mass of 1 mol $CaCO_3$ =		100.09 g

b. The exact amount is 486 g $CaCO_3$

Calcite crystals.

See Exercises 3.43 through 3.46

Sample Exercise 3.8

Molar Mass and Numbers of Molecules

Isopentyl acetate ($C_7H_{14}O_2$) is the compound responsible for the scent of bananas. A molecular model of isopentyl acetate is shown in the margin below. Interestingly, bees release about 1 μg (1×10^{-6} g) of this compound when they sting. The resulting scent attracts other bees to join the attack. How many molecules of isopentyl acetate are released in a typical bee sting? How many atoms of carbon are present?

Sample Exercise 3.8

Isopentyl acetate is released when a bee stings.

Solution

To find the number of molecules released in a sting, we must first determine the number of moles of isopentyl acetate in 1×10^{-6} g:

Sample Exercise 3.8

$$1 \times 10^{-6}\ \cancel{\text{g } C_7H_{14}O_2} = 8 \times 10^{-9}\ \text{mol } C_7H_{14}O_2$$

$$8 \times 10^{-9}\ \cancel{\text{mol } C_7H_{14}O_2} = 5 \times 10^{15}\ \text{molecules}$$

$$5 \times 10^{15}\ \cancel{\text{molecules}} = 4 \times 10^{16}\ \text{carbon atoms}$$

See Exercises 3.47 through 3.52

3.5 Percent Composition of Compounds

- There are two common ways of describing the composition of a compound: in terms of the numbers of its constituent atoms. The percentages (by mass) of its elements.
- For ethanol, which has the formula C_2H_5OH, the mass of each element present and the molar mass are obtained as follows:

$$\begin{aligned} \text{Mass of C} &= 24.02\ \text{g} \\ \text{Mass of H} &= 6.048\ \text{g} \\ \text{Mass of O} &= \underline{16.00\ \text{g}} \\ \text{Mass of 1 mol } C_2H_5OH &= 46.07\ \text{g} \end{aligned}$$

The **mass percent** (often called the weight percent) of carbon in ethanol can be computed by comparing the mass of carbon in 1 mole of ethanol to the total mass of 1 mole of ethanol and multiplying the result by 100:

$$\text{Mass percent of C} = \frac{\text{mass of C in 1 mol } C_2H_5OH}{\text{mass of 1 mol } C_2H_5OH} \times 100\%$$

$$\text{Mass percent of H} = 13.13\%$$

$$\text{Mass percent of O} = 34.73\%$$

Sample Exercise 3.10 Calculating Mass Percent Ⅱ

Penicillin, the first of a now large number of antibiotics (antibacterial agents), was discovered accidentally by the Scottish bacteriologist Alexander Fleming in 1928, but he was never able to isolate it as a pure compound. This and similar antibiotics have saved millions of lives that might have been lost to infections. Penicillin F has the formula $C_{14}H_{20}N_2SO_4$. Compute the mass percent of each element.

Sample Exercise 3.10

Solution

The molar mass of penicillin F is computed as follows:

C:	168.1 g
H:	120.16 g
N:	28.02 g
S:	32.07 g
O:	64.00 g

Mass of 1 mol $C_{14}H_{20}N_2SO_4$ = 312.4 g

Sample Exercise 3.10

Mass percent of C = 53.81%

Mass percent of H = 6.453%

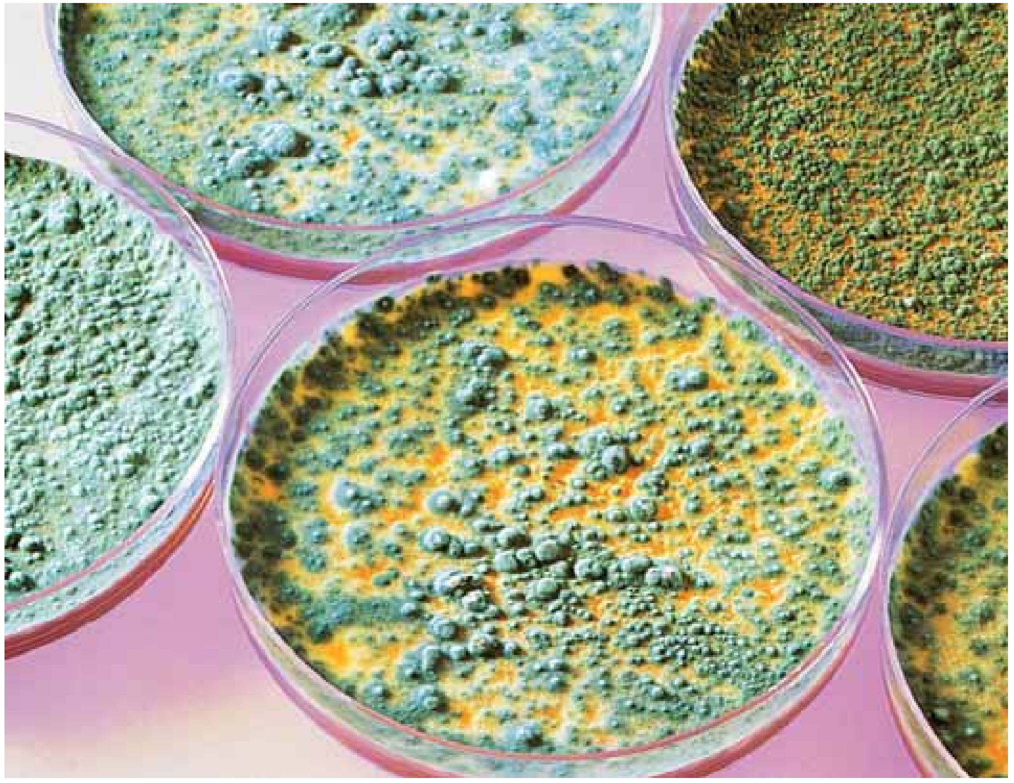
Mass percent of N = 8.969%

Mass percent of S = 10.27%

Mass percent of O = 20.49%

Reality Check: The percentages add up to 99.99%.

Sample Exercise 3.10



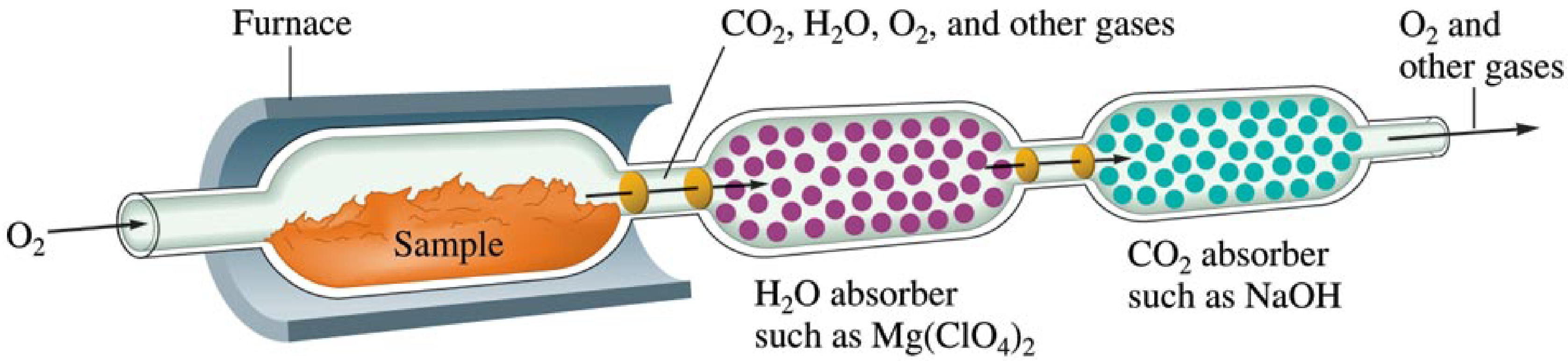
Penicillin is isolated from a mold that can be grown in large quantities in fermentation tanks.

See Exercises 3.61 and 3.62

3.6 Determining the Formula of a Compound

- A device is shown in Fig. 3.5.
- Suppose a substance has been prepared that is composed of carbon, hydrogen, and nitrogen. When 0.1156 gram of this compound is reacted with oxygen, 0.1638 gram of carbon dioxide (CO_2) and 0.1676 gram of water (H_2O) are collected.

Figure 3.5



A schematic diagram of the combustion device used to analyze substances for carbon and hydrogen. The sample is burned in the presence of excess oxygen, which converts all its carbon to carbon dioxide and all its hydrogen to water. These products are collected by absorption using appropriate materials, and their amounts are determined by measuring the increase in masses of the absorbents.

- The molar mass of CO_2 is

C:	12.01 g
O:	<u>32.00 g</u>
Molar mass of CO_2 =	44.01 g/mol

- The mass percent of carbon in this compound is 38.67% C.
- The molar mass of H_2O is 18.02 grams.

- The remainder must be nitrogen:

$$100.00\% - (\underbrace{38.67\%}_{\%C} + \underbrace{16.22\%}_{\%H}) = 45.11\%\ N$$

- In the present case, 38.67% carbon by mass means 38.67 grams of carbon per 100.00 grams of compound; 16.22% hydrogen means 16.22 grams of hydrogen per 100.00 grams of compound; and so on.

- To determine the formula, we must calculate the number of carbon atoms in 38.67 grams of carbon, the number of hydrogen atoms in 16.22 grams of hydrogen, and number of nitrogen atoms in 45.11 grams of nitrogen.
- We can find the smallest whole-number ratio of atoms in this compound :

C: 1
H: 5
N: 1

- Any molecule that can be represented as $(CH_5N)_n$, where is an integer, has the **empirical formula** CH_5N.
- To be able to specify the exact formula of the molecule involved, the **molecular formula**, we must know the molar mass.
- Suppose we know that this compound with empirical formula CH_5N has a molar mass of 31.06 g/mol.

$$1C:\quad 1 \times 12.01\ g = 12.01\ g$$

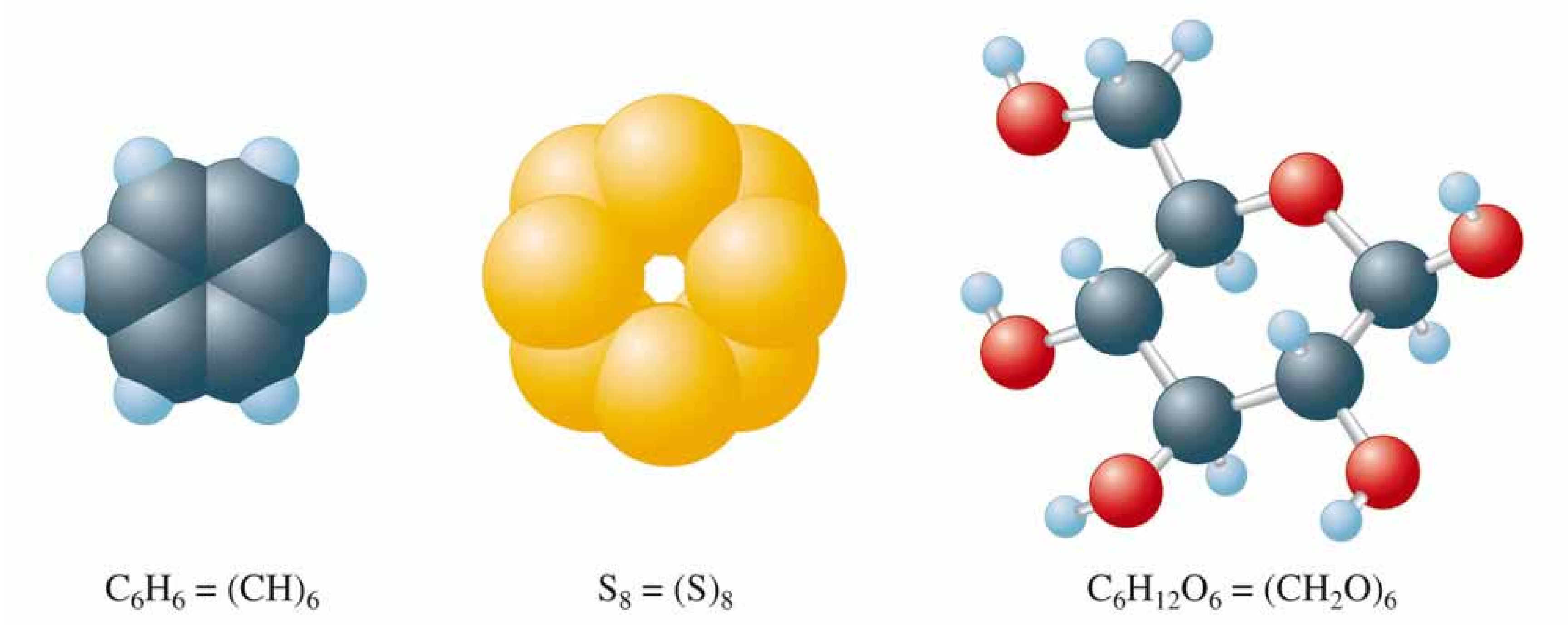
$$5H:\quad 5 \times 1.008\ g = 5.040\ g$$

$$1N:\quad 1 \times 14.01\ g = 14.01 g$$

$$\text{Formula mass of } CH_5N = 31.06\ g/mol$$

- Some examples where this is the case are shown in Fig. 3.6.

Figure 3.6



Examples of substances whose empirical and molecular formulas differ. Notice that molecular formula = (empirical formula)$_n$, where n is an integer.

Sample Exercise 3.11

Determining Empirical and molecule Formulas Ⅰ

Determine the empirical and molecular formulas for a compound that gives the following percentages upon analysis (in mass percent):

71.65% Cl   24.27% C   4.07% H

The molar mass is known to be 98.96 g/mol.

Solution

First, we convert the mass percents to masses in grams.

The molar mass is known to be 98.96 g/mol.

Sample Exercise 3.11

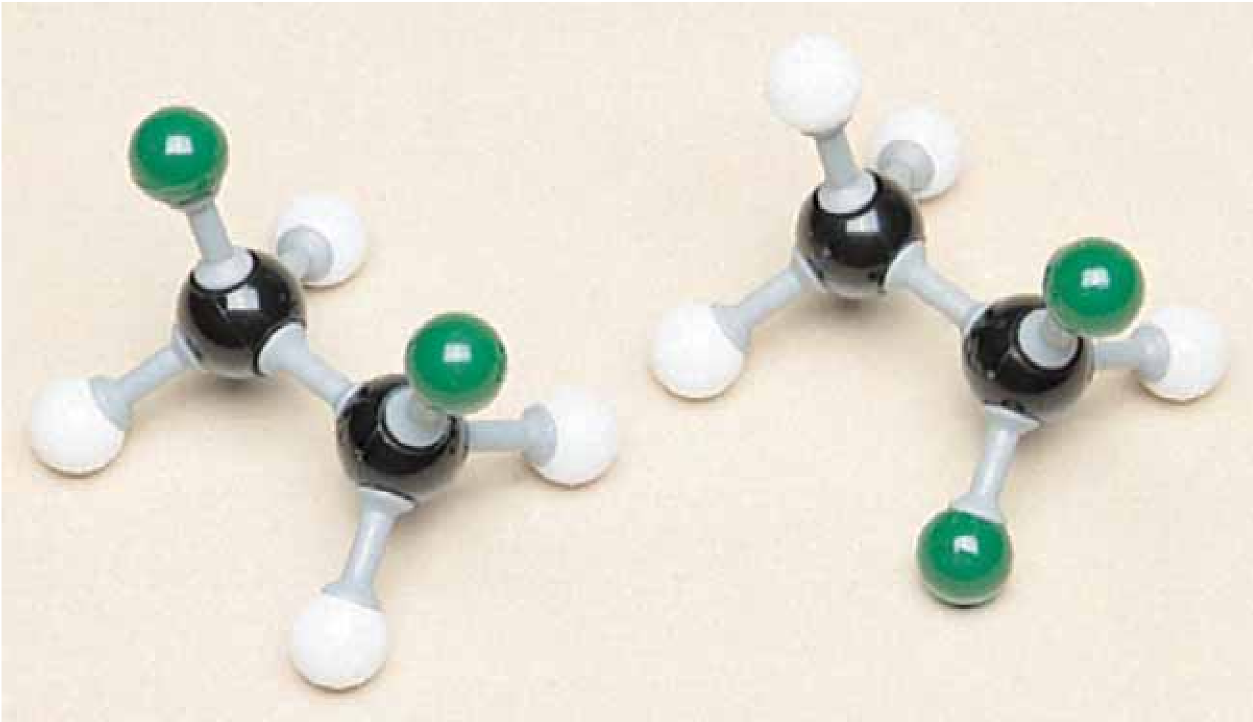
$$\frac{\text{Molar mass}}{\text{Empirical formula mass}} = \frac{98.96\ \text{g/mol}}{49.48\ \text{g/mol}} = 2$$

$$\text{Molecular formula} = (ClCH_2)_2 = Cl_2C_2H_4$$

The compound $C_{l2}C_2H_4$ is called *dichloroethane*. There are two forms of this compound, shown in Fig. 3.7.
The form on the right was formerly used as an additive in leaded gasoline

See Exercises 3.57 and 3.58

Figure 3.7



The two forms of dichloroethane.

Sample Exercise 3.12

Determining Empirical and molecule Formulas Ⅱ

A white powder is analyzed and found to contain 43.64% phosphorus and 56.36% oxygen by mass. The compound has a molar mass of 283.88 g/mol. What are the compound's empirical and molecular formulas?

Solution

In 100.00 g of this compound there are 43.64 g of phosphorus and 56.36 g of oxygen. In terms of moles, in 100.00 g of the compound we have

1.409 mol P and 3.523 mol O

Sample Exercise 3.12

$$\frac{1.409}{1.409} = 1\text{ P} \quad \text{and} \quad \frac{3.523}{1.409} = 2.5\text{ O}$$

This yields the formula $PO_{2.5}$. The empirical formula mass for P2O5 is 141.94.

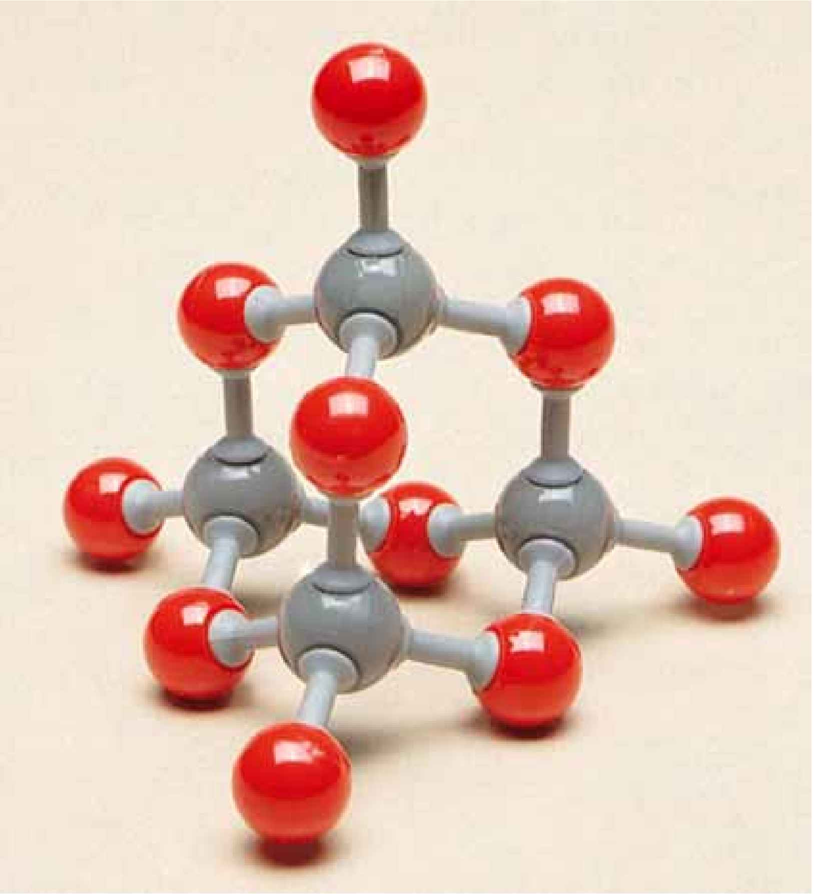
$$\frac{\text{Molar mass}}{\text{Empirical formula mass}} = \frac{283.88}{141.94} = 2$$

The molecular formula is $(P_2O_5)_2$, or P_4O_{10}. The structural formula of this interesting compound is given in Fig. 3.8.

See Exercises 3.59

Figure 3.8

The structure of P_4O_{10}. Note that some of the oxygen atoms act as “bridges” between the phosphorus atoms. This compound has a great affinity for water and is often used as a desiccant, or drying agent.



Empirical Formula Determination

- Since mass percentage gives the number of grams of a particular element per 100 grams of compound, base the calculation on 100 grams of compound. Each percent will then represent the mass in grams of that element.
- Determine the number of moles of each element present in 100 grams of compound using the atomic masses of the elements present.
- Divide each value of the number of moles by the smallest of the values. If each resulting number is a whole number (after appropriate rounding), these numbers represent the subscripts of the elements in the empirical formula.
- If the number obtained in the previous step are not whole numbers, multiply each number by an integer so that the results are all whole numbers.

Molecular Formula Determination

Method One

- Obtain the empirical formula.
- Compute the mass corresponding to the empirical formula.
- Calculate the ratio

$$\frac{\text{Molar mass}}{\text{Empirical formula mass}}$$

- The integer from the previous step represents the numbers of empirical formula units in one molecule. When the empirical formula subscripts are multiplied by this integer, the molecular formula results. This procedure is summarized by the equation:

$$\text{Molecular formula} = (\text{empirical formula}) \times \frac{\text{molar mass}}{\text{empirical formula mass}}$$

Method Two

- Using the mass percentages and the molar mass, determine the mass of each element present in one mole of compound.
- Determine the number of moles of each element present in one mole of compound.
- The integers from the previous step represent the subscripts in the molecular formula.