c. moles $C_{13}H_{18}O_2 \longrightarrow$ moles C $\longrightarrow$ grams C

To find the mass of carbon present in the ibuprofen, the two conversion factors needed are the amount of carbon in moles per mole of $C_{13}H_{18}O_2$ and the molar mass of carbon.

$$\text{mol } C_{13}H_{18}O_2 \times \frac{13 \text{ mol C}}{\text{mol } C_{13}H_{18}O_2} \times \frac{12.01 \text{ g C}}{\text{mol C}} = \text{g C}$$

3 SOLVE

a. $33 \text{ g } \cancel{C_{13}H_{18}O_2} \times \frac{1 \text{ mol } C_{13}H_{18}O_2}{206.31 \text{ g } \cancel{C_{13}H_{18}O_2}} = 0.16 \text{ mol } C_{13}H_{18}O_2$

b. $0.16\ \cancel{\text{mol}}\ C_{13}H_{18}O_2 \times \frac{6.022 \times 10^{23} \text{ molecules}}{\cancel{\text{mol}}} = 9.6 \times 10^{22} \text{ molecules } C_{13}H_{18}O_2$

c. $0.16\ \cancel{\text{mol } C_{13}H_{18}O_2} \times \frac{13\ \cancel{\text{mol C}}}{\cancel{\text{mol } C_{13}H_{18}O_2}} \times \frac{12.01 \text{ g C}}{\cancel{\text{mol C}}} = 25 \text{ g C}$

The bottle contains 0.16 mol of ibuprofen, which is 9.6×10^{22} molecules of ibuprofen.

The sample of ibuprofen contains 25 g of carbon.

4 CHECK YOUR WORK

Checking each step shows that the arithmetic is correct, significant figures have been used correctly, and units have canceled as desired.

Practice Answers in Appendix E

1. How many moles of compound are there in the following?
   - **a.** 6.60 g $(NH_4)_2SO_4$
   - **b.** 4.5 kg $Ca(OH)_2$
2. How many molecules are there in the following.
   - **a.** 25.0 g H_2SO_4
   - **b.** 125 g of sugar, $C_{12}H_{22}O_{11}$
3. What is the mass in grams of 6.25 mol of copper(II) nitrate?

MAIN IDEA

Percentage composition is the number of grams in one mole of a compound.

It is often useful to know the percentage by mass of a particular element in a chemical compound. For example, suppose the compound potassium chlorate, $KClO_3$, were to be used as a source of oxygen. It would be helpful to know the percentage of oxygen in the compound. To find the mass percentage of an element in a compound, one can divide the mass of the element in a sample of the compound by the total mass of the sample and then multiply this value by 100.

$$\frac{\text{mass of element in sample of compound}}{\text{mass of sample of compound}} \times 100 = \begin{array}{c}\text{\% element in}\\ \text{compound}\end{array}$$

The mass percentage of an element in a compound is the same regardless of the sample's size. Therefore, a simpler way to calculate the percentage of an element in a compound is to determine how many grams of the element are present in one mole of the compound. Then divide this value by the molar mass of the compound and multiply by 100.

$$\frac{\text{mass of element in 1 mol of compound}}{\text{molar mass of compound}} \times 100 = \begin{array}{l}\text{\% element in}\\ \text{compound}\end{array}$$

The percentage by mass of each element in a compound is known as the percentage composition of the compound.

Percentage Composition

Sample Problem J **Find the percentage composition of barium fluoride, BaF_2.**

1 ANALYZE

Given: formula, BaF_2

Unknown: percentage composition of BaF_2

2 PLAN

formula ⟶ molar mass ⟶ mass percentage of each element

The molar mass of the compound must be found. Then the mass of each element present in one mole of the compound is used to calculate the mass percentage of each element.

3 SOLVE

$$1\ \cancel{\text{mol Ba}} \times \frac{137.3\ \text{g Ba}}{\cancel{\text{mol Ba}}} = 137.3\ \text{g Ba}$$

$$2\ \cancel{\text{mol F}} \times \frac{18.99\ \text{g F}}{\cancel{\text{mol F}}} = 32.98\ \text{g F}$$

$$\text{molar mass of } BaF_2 = 175.3$$

$$\frac{137.3\ \text{g Ba}}{175.3\ \text{g } BaF_2} \times 100 = 78.32\%\ \text{Ba}$$

$$\frac{37.98\ \text{g F}}{175.3\ \text{g } BaF_2} \times 100 = 21.66\%\ \text{F}$$

4 CHECK YOUR WORK

A good check is to see if the results add up to about 100%. (Because of rounding, the total may not always be exactly 100%.)

Percentage Composition

Sample Problem K **As some salts crystallize from a water solution, they bind water molecules in their crystal structure. Sodium carbonate forms such a *hydrate*, in which 10 water molecules are present for every formula unit of sodium carbonate. Find the mass percentage of water in sodium carbonate decahydrate, $Na_2CO_3{\bullet}10H_2O$, which has a molar mass of 286.19 g/mol.**

Continued

Percentage Composition (continued)

1 ANALYZE

Given: chemical formula, $Na_2CO_3{\bullet}10H_2O$
molar mass of $Na_2CO_3{\bullet}10H_2O$

Unknown: mass percentage of H_2O

2 PLAN

chemical formula $\longrightarrow$ mass H_2O per mole of $Na_2CO_3{\bullet}10H_2O$ $\longrightarrow$ % water

The mass of water per mole of sodium carbonate decahydrate must first be found. This value is then divided by the mass of one mole of $Na_2CO_3{\bullet}10H_2O$.

3 SOLVE

One mole of $Na_2CO_3{\bullet}10H_2O$ contains 10 mol H_2O. As noted earlier, the molar mass of H_2O is 18.02 g/mol. The mass of 10 mol H_2O is calculated as follows.

$$10\ \cancel{\text{mol } H_2O} \times \frac{18.02\text{ g } H_2O}{\cancel{\text{mol } H_2O}} = 180.2\text{ g } H_2O$$

$$\text{mass of } H_2O \text{ per mole of } Na_2CO_3{\bullet}10H_2O = 180.2\text{ g}$$

The molar mass of $Na_2CO_3{\bullet}10H_2O$ is 286.19 g/mol, so we know that 1 mol of the hydrate has a mass of 286.19 g. The mass percentage of 10 mol H_2O in 1 mol $Na_2CO_3{\bullet}10H_2O$ can now be calculated.

$$\text{mass percentage of } H_2O \text{ in } Na_2CO_3{\bullet}10H_2O = \frac{180.2\text{ g } H_2O}{286.19\text{ g } Na_2CO_3{\bullet}10H_2O} \times 100$$

$$= 62.97\%\ H_2O$$

4 CHECK YOUR WORK

Checking shows that the arithmetic is correct and that units cancel as desired.

Practice

Answers in Appendix E

1. Find the percentage compositions of the following:
   a. C_3H_8 **b.** $NaHSO_4$
2. Find the mass percentage of water in $ZnSO_4{\bullet}7H_2O$.
3. Magnesium hydroxide is 54.87% oxygen by mass. How many grams of oxygen are in 175 g of the compound? How many moles of oxygen is this?

SECTION 3 FORMATIVE ASSESSMENT

Reviewing Main Ideas

1. Determine both the formula mass and molar mass of ammonium carbonate, $(NH_4)_2CO_3$.
2. How many moles of atoms of each element are there in one mole of $(NH_4)_2CO_3$?
3. What is the mass in grams of 3.25 mol $Fe_2(SO_4)_3$?
4. How many molecules of aspirin, $C_9H_8O_4$, are there in a 100.0 mg tablet of aspirin?
5. Calculate the percentage composition of $(NH_4)_2CO_3$.

Critical Thinking

6. **RELATING IDEAS** A sample of hydrated copper (II) sulfate ($CuSO_4{\bullet}nH_2O$) is heated to 150°C and produces 103.74 g anhydrous copper (II) sulfate and 58.55 g water. How many moles of water molecules are present in 1.0 mol of hydrated copper (II) sulfate?

SECTION 4

Main Ideas

- Empirical formulas show the whole-number ratio of elements in a compound.
- Molecular formulas give the types and numbers of atoms in a compound.

Determining Chemical Formulas

Key Terms

empirical formula

When a new substance is synthesized or is discovered, it is analyzed quantitatively to reveal its percentage composition. From these data, the empirical formula is then determined. **An empirical formula consists of the symbols for the elements combined in a compound, with subscripts showing the smallest whole-number mole ratio of the different atoms in the compound.** For an ionic compound, the formula unit is usually the compound's empirical formula. For a molecular compound, however, the empirical formula does not necessarily indicate the actual numbers of atoms present in each molecule. For example, the empirical formula of the gas diborane is BH_3, but the molecular formula is B_2H_6. In this case, the number of atoms given by the molecular formula corresponds to the empirical ratio multiplied by two.

MAIN IDEA

Empirical formulas show the whole-number ratio of elements in a compound.

To determine a compound's empirical formula from its percentage composition, begin by converting percentage composition to a mass composition. Assume that you have a 100.0 g sample of the compound. Then calculate the amount of each element in the sample. For example, the percentage composition of diborane is 78.1% B and 21.9% H. Therefore, 100.0 g of diborane contains 78.1 g of B and 21.9 g of H.

Next, convert the mass composition of each element to a composition in moles by dividing by the appropriate molar mass.

$$78.1\ \cancel{\text{g B}} \times \frac{1\ \text{mol B}}{10.81\ \cancel{\text{g B}}} = 7.22\ \text{mol B}$$

$$21.9\ \cancel{\text{g H}} \times \frac{1\ \text{mol H}}{1.01\ \cancel{\text{g H}}} = 21.7\ \text{mol H}$$

These values give a mole ratio of 7.22 mol B to 21.7 mol H. However, this is not a ratio of least whole numbers. To find such a ratio, divide each number of moles by the least number in the existing ratio.

$$\frac{7.22\ \text{mol B}}{7.22} : \frac{21.7\ \text{mol H}}{7.22} = 1\ \text{mol B} : 3.01\ \text{mol H}$$

Because of rounding or experimental error, a compound's mole ratio sometimes consists of numbers close to whole numbers instead of exact whole numbers. In this case, the differences from whole numbers may be ignored and the nearest whole number taken. Thus, diborane contains atoms in the ratio 1 B : 3 H. The compound's empirical formula is BH_3.

Sometimes mass composition is known instead of percentage composition. To determine the empirical formula in this case, convert mass composition to composition in moles. Then calculate the least whole-number mole ratio of atoms. This process is shown in Sample Problem M.

Empirical Formulas

Sample Problem L **Quantitative analysis shows that a compound contains 2.016% hydrogen, 32.60% sulfur, and 65.30% oxygen. Find the empirical formula of this compound.**

1 ANALYZE

Given: percentage composition: 2.016% H, 32.60% S, and 65.30% O

Unknown: empirical formula

2 PLAN

percentage composition ⟶ mass composition ⟶ composition in moles ⟶ least whole-number mole ratio of atoms

3 SOLVE

Mass composition (mass of each element in 100.0 g sample):
2.016 g H, 32.60 g S, and 65.30 g O

$$\text{Composition in moles:}\quad 2.016\ \text{g}\,\cancel{\text{H}} \times \frac{1\ \text{mol H}}{1.007\ \text{g}\,\cancel{\text{H}}} = 2.001\ \text{mol H}$$

$$32.60\ \text{g}\,\cancel{\text{S}} \times \frac{1\ \text{mol S}}{32.06\ \text{g}\,\cancel{\text{S}}} = 1.016\ \text{mol S}$$

$$65.30\ \text{g}\,\cancel{\text{O}} \times \frac{1\ \text{mol O}}{16.00\ \text{g}\,\cancel{\text{O}}} = 4.081\ \text{mol O}$$

Least whole-number mole ratio of atoms:
The compound contains atoms in the ratio 2.001 mol H : 1.016 mol S : 4.081 mol O. To find the least whole-number mole ratio, divide each value by the least number in the ratio.

$$\frac{2.001\ \text{mol H}}{1.016} : \frac{1.016\ \text{mol S}}{1.016} : \frac{4.081\ \text{mol O}}{1.016} = 1.969\ \text{mol H} : 1\ \text{mol S} : 4.019\ \text{mol O}$$

Rounding each number in the ratio to the nearest whole number yields a mole ratio of 2 mol H : 1 mol S : 4 mol O. The empirical formula of the compound is H_2SO_4.

4 CHECK YOUR WORK

Calculating the percentage composition of the compound based on the empirical formula determined in the problem reveals a percentage composition of 1.008% H, 32.69% S, and 65.24% O. These values agree reasonably well with the given percentage composition.

GO ONLINE

Solve It! Cards
HMHScience.com

Empirical Formulas

Sample Problem M **Analysis of a 10.150 g sample of a compound known to contain only phosphorus and oxygen indicates a phosphorus content of 4.433 g. What is the empirical formula of this compound?**

1 ANALYZE

Given: sample mass = 10.150 g

phosphorus mass = 4.433 g

Unknown: empirical formula

2 PLAN

Mass composition ⟶ composition in moles ⟶ smallest whole-number ratio of atoms

3 SOLVE

The mass of oxygen is found by subtracting the phosphorus mass from the sample mass.

$$\text{sample mass} - \text{phosphorus mass} = 10.150 \text{ g} - 4.433 \text{ g} = 5.717 \text{ g}$$

Mass composition: 4.433 g P, 5.717 g O

Composition in moles:

$$4.433 \cancel{\text{g P}} \times \frac{1 \text{ mol P}}{30.97 \cancel{\text{g P}}} = 0.1431 \text{ mol P}$$

$$5.717 \cancel{\text{g O}} \times \frac{1 \text{ mol O}}{16.00 \cancel{\text{g O}}} = 0.3573 \text{ mol O}$$

Least whole-number mole ratio of atoms:

$$\frac{0.1431 \text{ mol P}}{0.1431} : \frac{0.3573 \text{ mol O}}{0.1431}$$

$$1 \text{ mol P} : 2.497 \text{ mol O}$$

The number of O atoms is not close to a whole number. But if we multiply each number in the ratio by 2, then the number of O atoms becomes 4.994 mol, which is close to 5 mol. The least whole-number mole ratio of P atoms to O atoms is 2 : 5. The compound's empirical formula is P_2O_5.

4 CHECK YOUR WORK

The arithmetic is correct, significant figures have been used correctly, and units cancel as desired. The formula is reasonable because +5 is a common oxidation state of phosphorus.

Practice Answers in Appendix E

1. A compound is found to contain 6.1% hydrogen and 93.9% oxygen. Find its empirical formula.
2. Find the empirical formula of a compound found to contain 26.56% potassium, 35.41% chromium, and the remainder oxygen.
3. Analysis of 20.0 g of a compound containing only calcium and bromine indicates that 4.00 g of calcium are present. What is the empirical formula of the compound formed?

MAIN IDEA

Molecular formulas give the types and numbers of atoms in a compound.

Remember that the *empirical formula* contains the least possible whole numbers that describe the atomic ratio. The *molecular formula* is the actual formula of a molecular compound. An empirical formula may or may not be a correct molecular formula. For example, diborane's empirical formula is BH_3. Any multiple of BH_3, such as B_2H_6, B_3H_9, B_4H_{12}, and so on, represents the same ratio of B atoms to H atoms. The molecular compounds ethene, C_2H_4, and cyclopropane, C_3H_6, also share an identical atomic ratio (2 H : 1 C), yet they are very different substances. How is the correct formula of a molecular compound found from an empirical formula?

The relationship between a compound's empirical formula and its molecular formula can be written as follows.

$$x\text{(empirical formula)} = \text{molecular formula}$$

The number represented by x is a whole-number multiple indicating the factor by which the subscripts in the empirical formula must be multiplied to obtain the molecular formula. (The value of x is sometimes 1.) The formula masses have a similar relationship.

$$x\text{(empirical formula mass)} = \text{molecular formula mass}$$

To determine the molecular formula of a compound, you must know the compound's formula mass. For example, experimentation shows the formula mass of diborane to be 27.67 u. The formula mass for the empirical formula, BH_3, is 13.84 u. Dividing the experimental formula mass by the empirical formula mass gives the value of x for diborane.

$$x = \frac{27.67\text{ u}}{13.84\text{ u}} = 2.000$$

The molecular formula of diborane is therefore B_2H_6.

$$2(BH_3) = B_2H_6$$

Recall that a compound's molecular formula mass is numerically equal to its molar mass, so a compound's molecular formula can also be found given the compound's empirical formula and its molar mass.

Molecular Formulas

Sample Problem N **In Sample Problem M, the empirical formula of a compound of phosphorus and oxygen was found to be P_2O_5. Experimentation shows that the molar mass of this compound is 283.89 g/mol. What is the compound's molecular formula?**

1 ANALYZE

Given: empirical formula

Unknown: molecular formula

Continued

2 PLAN

$$x\,(\text{empirical formula}) = \text{molecular formula}$$

$$x = \frac{\text{molecular formula mass}}{\text{empirical formula mass}}$$

3 SOLVE

Molecular formula mass is numerically equal to molar mass. Thus, changing the g/mol unit of the compound's molar mass to u yields the compound's molecular formula mass.

$$\text{molecular molar mass} = 283.89 \text{ g/mol}$$
$$\text{molecular formula mass} = 283.89 \text{ u}$$

The empirical formula mass is found by adding the masses of each of the atoms indicated in the empirical formula.

$$\text{mass of phosphorus atom} = 30.97 \text{ u}$$
$$\text{mass of oxygen atom} = 16.00 \text{ u}$$
$$\text{empirical formula mass of } P_2O_5 = 2 \times 30.97 \text{ u} + 5 \times 16.00 \text{ u} = 141.94 \text{ u}$$

Dividing the experimental formula mass by the empirical formula mass gives the value of x. The formula mass is numerically equal to the molar mass.

$$x = \frac{283.89 \cancel{\text{ u}}}{141.94 \cancel{\text{ u}}} = 2.0001$$

The compound's molecular formula is therefore P_4O_{10}.

$$2 \times (P_2O_5) = P_4O_{10}$$

4 CHECK YOUR WORK

Checking the arithmetic shows that it is correct.

Practice Answers in Appendix E

1. Determine the molecular formula of the compound with an empirical formula of CH and a formula mass of 78.110 u.
2. A sample of a compound with a formula mass of 34.00 u is found to consist of 0.44 g H and 6.92 g O. Find its molecular formula.

SECTION 4 FORMATIVE ASSESSMENT

Reviewing Main Ideas

1. A compound contains 36.48% Na, 25.41% S, and 38.11% O. Find its empirical formula.
2. Find the empirical formula of a compound containing 53.70% iron and 46.30% sulfur.
3. Analysis of a compound indicates that it contains 1.04 g K, 0.70 g Cr, and 0.86 g O. Find its empirical formula.
4. If 4.04 g of N combine with 11.46 g O to produce a compound with a formula mass of 108.0 u, what is the molecular formula of this compound?

Critical Thinking

5. **RELATING IDEAS** A compound containing sodium, chlorine, and oxygen is 25.42% sodium by mass. A 3.25 g sample gives 4.33×10^{22} atoms of oxygen. What is the empirical formula?