3.8: The Mole Concept for Compounds

The molar mass of a compound is the sum of the atomic masses of all of the elements in the formula.

For molecular compounds, this is the mass of one mole of molecules, and for ionic compounds it is the mass of one mole of formula units.

Example: How many moles and total number of molecules are in 22.7 g C_2H_6O?

First calculate the molar mass of C_2H_6O:

$2 \times$ MM of C + $6 \times$ MM of H + $1 \times$ MM of O

$2 \times 12.01\ g/mol + 6 \times 1.008\ g/mol + 1 \times 16.00\ g/mol$

$= 46.07\ g/mol$

$$\frac{22.7\ g}{46.07\ g/mol} = 0.493\ mol$$

$$0.493\ mol \times 6.022 \times 10^{23}\ \frac{molecules}{mol}$$

$= 2.97 \times 10^{23}$ molecules

3.9: Composition of Compounds

The **percent composition** of a compound is the percentage of the total mass of the compound that is due to the mass of each element.

The percent by mass of each element in a compound can be calculated by this formula:

$$\%\text{ of element} = \frac{n \times \text{molar mass of the element}}{\text{molar mass of the compound}} \times 100$$

Where n is the number of moles of the element in 1 mol of the compound (*i.e.* its subscript in the formula of the compound)

Example: What is the percent composition of C_2H_6O?

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$$\% C = \frac{2 \times 12.01 \text{ g/mol}}{46.07 \text{ g/mol}} \times 100 = 52.14\%$$

$$\% H = \frac{6 \times 1.008 \text{ g/mol}}{46.07 \text{ g/mol}} \times 100 = 13.13\%$$

$$\% O = \frac{1 \times 16.00 \text{ g/mol}}{46.07 \text{ g/mol}} \times 100 = 34.73\%$$

Types of Chemical Formulas

Acetylene C_2H_2 - Molecular formula

simplest ratio CH - Empirical formula

Section 3.10: Determining a Chemical Formula from Experimental Data

The empirical formula of a compound can be calculated from its percent composition.

Example: Analysis of lactic acid shows that it is 40.0 % C, 6.71 % H and 53.3 % O by mass. What is the empirical formula of lactic acid?

Usually it is most convenient to assume there is 100 g total **of the compound, since then the percentages become grams** (note that the % composition is the same for any amount of compound):

40.0 g C 6.71 g H 53.3 g O

The **empirical formula** of a compound is the simplest whole number ratio of its elements.

The formula of an ionic compound (*e.g.* NaCl) gives the composition of its **formula unit**, the simplest whole number ratio of ions (so it is really an empirical formula).

Convert grams to moles:

ratio:

$\frac{40.0\text{ g C}}{12.01\text{ g/mol}} = 3.331\text{ mol C}$ 1

$\frac{6.71\text{ g H}}{1.008\text{ g/mol}} = 6.644\text{ mol H}$ 2

$\frac{53.3\text{ g O}}{16.00\text{ g/mol}} = 3.331\text{ mol O}$ 1

empirical formula: CH_2O

What is the molecular formula of lactic acid?

It must be a multiple of the empirical formula.

could be: $CH_2O \times 1 = CH_2O$
$CH_2O \times 2 \quad C_2H_4O_2$
$\times 3 \quad C_3H_6O_3$
$\times 4 \quad C_4H_8O_4$

Need to know the molar mass:
90.08 g/mol for lactic acid

"empirical formula mass"

CH_2O - 30.03 g/mol

$\frac{90.08}{30.03} = 3$ Molecular formula is 3 × empirical formula

$CH_2O \times 3 = \boxed{C_3H_6O_3}$

Summary:

Given the percent composition of a compound:

1. Assume 100 g total, so percentages become grams.
2. Convert grams of each element to moles.
3. Look for the simplest whole number ratio of moles; this is the empirical formula of the compound.
4. Use the empirical formula, and the molar mass of the compound, to calculate the molecular formula

What if the empirical formula cannot be determined from the number of moles of each element *by inspection*?

You can follow this procedure:

1. Divide each number of moles by the smallest number of moles.
2. If some of the moles are still not whole numbers, multiply each number by the smallest factor that will give all integers (see table at bottom of p. 115 of textbook).

For example see the calculation of the empirical formula of aspirin, Example 3.18 on p.115 of the textbook. You can watch a video in which this example is worked. The link is just below the link for this pencast.

Fractional Subscript	Multiply by This
0.20	5
0.25	4
0.33	3
0.40	5
0.50	2
0.66	3
0.75	4
0.80	5