3. Avogadro's Number and the Molar Mass of an Element

In the SI system the mole (mol) is the amount of a substance that contains as many elementary entities (atoms, molecules, or other particles) as there are atoms in exactly 12 g (or 0.012 kg) of the carbon-12 isotope. The actual number of atoms in 12 g of carbon-12 is called **Avogadro's Number (N_A)**, in an honor of the Italian scientist Amadeo Avogadro, currently accepted value is

$$\mathbf{N_A = 6.0221415 \times 10^{23}}$$

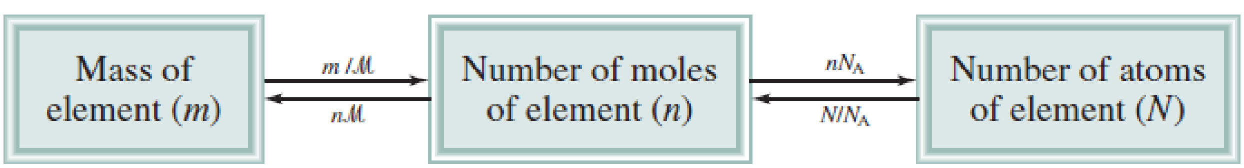
$$\mathbf{1 \text{ mole of } X = 6.022 \times 10^{23} \text{ units of } X}$$

Thus, just as one mole of hydrogen atoms contains 6.022×10^{23} H atoms.

We have seen that 1 mole of carbon-12 atoms has a mass of exactly 12 g and contains 6.022×10^{23} atoms. This mass of carbon-12 is its **molar mass ($\mathcal{M}$)**, defined as **the mass (in grams or kilograms) of 1 mole of units** (such as atoms or molecules) of a substance. Likewise, the atomic mass of sodium (N_a) is 22.99 amu and its molar mass is 22.99 g; the atomic mass of phosphorus is 30.97 amu and its molar mass is 30.97 g; and so on.

Knowing the molar mass and Avogadro's number, we can calculate the mass of a single atom in grams. For example, we know the molar mass of carbon-12 is 12.00 g and there are 6.022×10^{23} carbon-12 atoms in 1 mole of the substance; therefore, the mass of one carbon-12 atom is given by

$$\frac{12.00 \text{ g carbon}-12 \text{ atoms}}{6.022 \times 10^{23} \text{ carbon}-12 \text{ atoms}} = 1.993 \times 10^{-23} \text{ g}$$



The relationship between mass (m in grams) of an element and number of moles of an elements (n) and between number of moles of an element and number of atoms (N) of an element. $\mathcal{M}$ is the molar mass (g/mol) of the element and N_A is Avogadro's number.

We can use the preceding result to determine the relationship between atomic mass units and grams. Because the mass of every carbon-12 atom is exactly 12 amu, the number of atomic mass unit equivalent to 1 gram is

The **percent composition by mass** is the percent by mass of each element in a compound. Percent composition is obtained by dividing the mass of each element in 1 mole of the compound by the molar mass of the compound and multiplying by 100 percent.

$$\text{Percent composition of an element} = \frac{n \; x \; molar \; mass \; of \; element}{molar \; mass \; of \; compound} \text{ x } 100\%$$

Where n is the number of moles of the element in 1 mole of the compound. For example, in 1 mole of hydrogen peroxide (H_2O_2) there are 2 moles of H atoms and 2 moles of O atoms. The molar masses of H_2O_2, H, and O are 34.02 g, 1.008 g, and 16.00 g, respectively. Therefore, the percent composition of H_2O_2 is calculated as follows:

$$\% \text{ H} = \frac{2 \; x \; 1.008 \; g \; H}{34.02 \; g \; H_2O_2} \text{ x } 100\% = 5.926\%$$

$$\% \text{ O} = \frac{2 \; x \; 16.00 \; g \; O}{34.02 \; g \; H_2O_2} \text{ x } 100\% = 94.06\%$$

The sum of percentages is 5.926% + 94.06% = 99.99%. The small of discrepancy from 100 percent is due to the way we rounded off the molar masses of the elements.

Example

Analysis of a 12.04 g sample of a liquid compound composed of carbon, hydrogen, and nitrogen showed it tto contain 7.34 g C, 1.85 g H, and 2.85 g N. **What is the percent composition of this compound?**

Solution

To calculate percent composition, we divide the experimentally derived mass of each element by the overall mass of the compound, and then convert to a percentage:

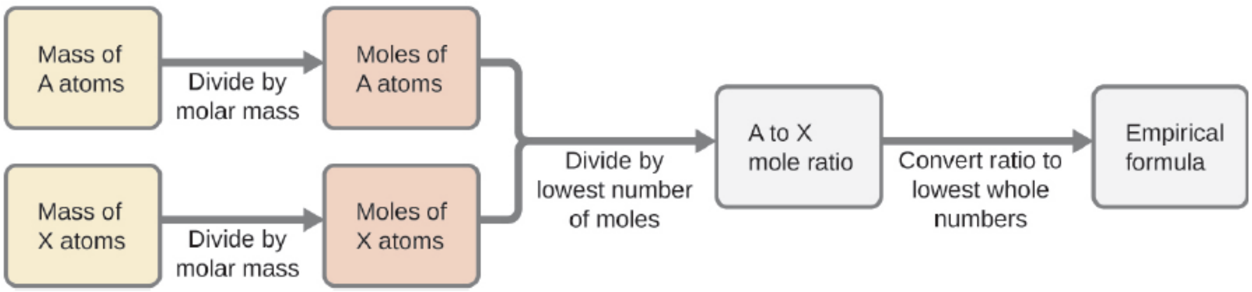
$$\%\text{C} = \frac{7.34 \; g \; C}{12.04 \; g \; compound} \text{ x } 100\% = 61.0\%$$

$$\%\text{H} = \frac{1.85 \; g \; H}{12.04 \; g \; compound} \text{ x } 100\% = 15.4\%$$

$$\%\text{N} = \frac{2.85 \; g \; N}{12.04 \; g \; compound} \text{ x } 100\% = 23.7\%$$

In summary, empirical formulas are derived from experimentally measured element masses by:

1. Deriving the number of moles of each element from its mass
2. Dividing each element's molar amount by the smallest molar amount to yield subscripts for a tentative empirical formula
3. Multiplying all coefficients by an integer, if necessary, to ensure that the smallest whole-number ratio of subscripts is obtained



Derivation of Molecular Formulas

Molecular formula are derived by comparing the compound's molecular or molar mass to its empirical formula mass. Empirical formula mass is the sum of the average atomic masses of all the atoms represented in an empirical formula. If we know the molecular (or molar) mass of the substance, we can divide this by the empirical formula mass in order to identify the number of empirical formula units per molecule, which we designate as ***n***:

$$\frac{\text{molecular or molar mass (amu or } \frac{g}{mol}\text{)}}{\text{empirical formula mass (amu or } \frac{g}{mol}\text{)}} = \text{n formula units/molecule}$$

The molecular formula is then obtained by multiplying each subscript in the empirical formula by ***n***, as shown by the generic empirical formula A_xB_y:

$$(A_xB_y)_n = A_{nx}B_{nx}$$

For example, consider a covalent compound whose empirical formula is determined to be CH_2O. The empirical formula mass for this compound is approximately 30 amu(the sum of 12 amu for one C atom, 2 amu for two H atoms, and 16 amu for one O atom). If the compound molecular mass is determined to be 180 amu, this indicates that molecules of this compound contain six times the number of atoms represented in the empirical formula:

Example

When aluminum metal is exposed to air, a protective layer of aluminum oxide (Al_2O_3) forms on its surface. This layer prevents further reaction between aluminum and oxygen, and it's the reason that aluminum beverage cans do not corrode. **Write a balance equation for the formation of Al_2O_3**.

Solution

The unbalance equation is

$$Al + O_2 \longrightarrow Al_2O_3$$

We see that there is one Al atom on the reactants side and there are two Al atoms on the product side. We can balance the Al atoms by placing a coefficient of 2 in front of Al on the reactants side.

$$2\,Al + O_2 \longrightarrow Al_2O_3$$

There are two O atoms on the reactants side, and three O atoms on the product side of the equation. We can balance the O atoms by placing a coefficient of $\frac{3}{2}$ in front of O_2 on the reactant side.

$$2\,Al + \frac{3}{2}O_2 \longrightarrow Al_2O_3$$

This is a balance equation. However, equations are normally balanced with the smallest set of whole number coefficients. Multiplying both sides of the equation by 2 gives whole number coefficients.

$$2\,(2\,Al + \frac{3}{2}O_2 \longrightarrow Al_2O_3)$$

or

$$\mathbf{4\,Al + 3\,O_2 \longrightarrow 2\,Al_2O_3}$$

Equations for Ionic Reactions

When aqueous solutions of $CaCl_2$ and $AgNO_3$ are mixed, a reaction takes place producing aqueous $Ca(NO_3)_2$ and solid $AgCl_2$.

$CaCl_2(aq) + 2\,AgNO_3(aq) \longrightarrow Ca(NO_3)_2(aq) + 2\,AgCl(s)$

$$\text{charge on } SO_3^{2-} = -2 = (3 \times (-2)) + (1 \times S)$$

$$\mathbf{S = -2 - (3 \times (-2)) = +4}$$

c. For ionic compounds, it's convenient to assign oxidation numbers for the cation and anion separately.
According to guideline 2, the oxidation number for sodium is +1.
Assuming the usual oxidation number for oxygen (–2 per guideline 3), the oxidation number for sulfur is calculated as directed by guideline 4:

$$\text{charge on } SO_4^{2-} = -2 = (4 \times (-2)) + (1 \times S)$$

$$\mathbf{S = -2 - (4 \times (-2)) = +6}$$

Oxidation-reduction (redox) reactions are those in which one or more elements involved undergo a change in oxidation number. Definition for the complementary process of this reaction class are correspondingly revised as:

oxidation = increase in oxidation number

reduction = decrease in oxidation number

In the reaction between sodium and chlorine to yield sodium chloride, sodium is oxidized (its oxidation number increases from 0 in Na^+ to 1 in NaCl) and chlorine is reduced (its oxidation number decreases from 0 in Cl_2 to –1 in NaCl). In the reaction between molecular hydrogen and chlorine, hydrogen is oxidized (its oxidation number increases from 0 in H_2O to +1 in HCl) and chlorine is reduced (its oxidation number decreases from 0 in Cl_2 to -1 in HCl).

Example

Identify which equations represent redox reactions, providing a name for the reaction if appropriate. For those reactions identified as redox, name the oxidant and reductant.

a. $ZnCO_3(s) \longrightarrow ZnO(s) + CO_2(g)$

b. $2\,Ga(l) + 3\,Br_2(l) \longrightarrow 2\,GaBr_3(s)$

c. $2\,H_2O_2(aq) \longrightarrow 2\,H_2O(l) + O_2(g)$

d. $BaCl_2(aq) + K_2SO_4(aq) \longrightarrow BaSO_4(s) + 2\,KCl(aq)$

e. $C_2H_4(g) + 3\,O_2(g) \longrightarrow 2\,CO_2(g) + 2\,H_2O(l)$

Solution

a. This is not redox reaction, since oxidation numbers remain unchanged for all elements.
b. This is a redox reaction. Gallium is oxidized, its oxidation number increasing from 0 in Ga(l) to +3 in $GaBr_3$(s). The reducing agent is Ga(l). Bromine is reduced, its oxidation number decreasing from 0 in Br_2(l) to –1 in $GaBr_3$(s). The oxidizing agent is Br_2(l).
c. This is a redox reaction. It involves the same element, oxygen, undergoing both oxidation and reduction (a so-called **disproportionation reaction**). Oxygen is oxidized, its oxidation number increasing from –1 in H_2O_2(aq) to 0 in O_2(g). Oxygen is also reduced, its oxidation number decreasing from –1 in H_2O_2(aq) to –2 in H_2O(l). For disproportionation reactions, the same substance functions as an oxidant and a reductant.
d. This is not redox reaction, since oxidation numbers remain unchanged for all elements.
e. This is a redox reaction (combustion). Carbon is oxidized, its oxidation number increasing from –2 in C_2H_4(g) to +4 in CO_2(g). The reducing agent (fuel) is C_2H_4(g). Oxygen is reduced, its oxidation number decreasing from 0 in O_2(g) to –2 in H_2O(l). The oxidizing agent is O_2(g).

Balancing Redox Reactions via the Half-Reaction Method

Redox reactions that take place in aqueous media often involve water, hydronium ions, and hydroxide ions as reactants or products. Although this species are not oxidizes or reduced, they do participate in chemical change in other ways (e.g., by providing the elements required to form oxyanions). Equation representing these reactions are sometimes very difficult to balance by inspection, so systematic approach have been developed to assist in the process. One very useful approach is to use the method of half-reactions, which involves the following steps:

1. Write the two half-reactions representing the redox process.
2. Balance all elements except oxygen and hydrogen.
3. Balance oxygen atoms by adding H_2O molecules.
4. Balance hydrogen atoms by adding H^+ ions.
5. Balance charge by adding electrons.
6. If necessary, multiply each half-reaction's coefficients by the smallest possible integers to yield equal numbers of electrons in each.

9. Reaction Stoichiometry

A balanced chemical equation provides a great deal of information in a very succinct format. Chemical formulas provide the identities of the reactants and products involved in the chemical change, allowing classification of the reaction. Coefficient provide the relative numbers of these chemical species, allowing a quantitative assessment of the relationships between the amounts of substances consumed and produced by the reaction. These quantitative relationships are known as the reaction's **stoichiometry**.

Balance chemical equations are used in much the same fashion to determine the amount of one reactant required to react with a given amount of another reactant, or to yield a given amount of product, and so forth. The coefficients in the balance equation are used to derived **stoichiometric factors** that permit computation of the desired quantity. To illustrate this idea, consider the production of ammonia by reaction of hydrogen and nitrogen:

$$N_2(g) + 3\,H_2(g) \longrightarrow 2\,NH_3(g)$$

This equation shows ammonia molecules are produced from hydrogen molecules in a 2:3 ratio, and stoichiometric factors may be derived using any amount (number) unit:

$$\frac{2\ \mathrm{NH_3\ molecules}}{3\ \mathrm{H_2\ molecules}} \text{ or } \frac{2\ \mathrm{doz\ NH_3\ molecules}}{3\ \mathrm{doz\ H_2\ molecules}} \text{ or } \frac{2\ \mathrm{mol\ NH_3\ molecules}}{3\ \mathrm{mol\ H_2\ molecules}}$$

These stoichiometric factors can be used to compute the number of ammonia molecules produced from a given number of hydrogen molecules, or the number of hydrogen molecules required to produce a given number of ammonia molecules.

Numerous variations on the beginning and ending computational steps are possible depending upon what particular quantities are provided and sought (volumes, solution concentration, and so forth). Figure below provide a general outline of the various computational steps associated with many reaction stoichiometry calculations.