1. Moles : In chemistry, a mole is a unit used to count particles like atoms, molecules, or ions.

$$\text{Moles} = \frac{Mass\ (g)}{Molar\ mass\ (\frac{g}{mol})}$$

$$\mathbf{n} = \frac{\boldsymbol{m}}{\boldsymbol{M}}$$

2. Density: is a measure of how much mass is packed into a given volume.

$$\text{Density} = \frac{Mass}{Volume}$$

$$\boldsymbol{\rho} = \frac{\boldsymbol{m}}{\boldsymbol{v}}$$

3. Concentration: tells us how much solute (like salt or sugar) is dissolved in a solvent (like water).

$$\text{Concentration} = \frac{Moles\ of\ solute}{volume\ of\ solution}$$

$$\text{M} = \frac{n(mol)}{v(l)}$$

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In the SI system a mole is composed of 6.022×10^{23} (**Avogadro's number**) molecules. To convert the number of moles to mass and the mass to moles, we make use of the **molecular weight** – the mass per mole:

$$\text{Molecular Weight (MW)} = \frac{\text{Mass}}{\text{Mole}}$$

Thus, the calculations you carry out are

$$\text{the g mol} = \frac{\text{mass in g}}{\text{molecular weight}}$$

$$\text{the lb mol} = \frac{\text{mass in lb}}{\text{molecular weight}}$$

and

$$\text{Mass in g} = (\text{MW})(\text{g mol})$$

$$\text{Mass in lb} = (\text{MW})(\text{lb mol})$$

For example

$$\frac{100.0 \text{ g } H_2O}{} \left| \frac{1 \text{ g mol } H_2O}{18.0 \text{ g } H_2O} \right. = 5.56 \text{ g mol } H_2O$$

$$\frac{6.0 \text{ lb mol } O_2}{} \left| \frac{32.0 \text{ lb } O_2}{1 \text{ lb mol } O_2} \right. = 192 \text{ lb } O_2$$

Example 2.10 Use of Molecular Weights to Convert Moles to Mass

How many pounds of NaOH are in 7.50 g mol of NaOH?

Solution

This problem involves converting gram moles to pounds. From Example 2.9, the MW of NaOH is 40.0:

$$\frac{7.50 \text{ g mol NaOH}}{} \left| \frac{1 \text{ lb mol}}{454 \text{ g mol}} \right| \frac{40.0 \text{ lb NaOH}}{1 \text{ lb mol NaOH}} = 0.661 \text{ lb NaOH}$$

Note the conversion between pound moles and gram moles was to proceed from SI to the AE system of units. Could you first convert 7.50 g mol of NaOH to grams of NaOH, and then use the conversion of 454g = 1 lb to get pounds of NaOH? Of course.

Example 2.9 Use of Molecular Weights to Convert Mass to Moles

If a bucket holds 2.00 lb of NaOH:

a. How many pound moles of NaOH does it contain?
b. How many gram moles of NaOH does it contain?

Solution

You can convert pounds to pound moles, and then convert the values to the SI system of units. Look up the molecular weight of NaOH, or calculate it from the atomic weights. (It is 40.0.) Note that the molecular weight is used as a conversion factor in this calculation:

$$\textbf{a.}\quad \frac{2.00 \text{ lb NaOH}}{} \left| \frac{1 \text{ lb mol NaOH}}{40.0 \text{ lb NaOH}} \right. = 0.050 \text{ lb mol NaOH}$$

$$\textbf{b1.}\quad \frac{2.00 \text{ lb NaOH}}{} \left| \frac{1 \text{ lb mol NaOH}}{40.0 \text{ lb NaOH}} \right| \frac{454 \text{ g mol}}{1 \text{ lb mol}} = 22.7 \text{ g mol}$$

Example 2.11 Average Molecular Weight of Air

Calculate the average molecular weight of air, assuming that air is 21% O_2 and 79% N_2.

Solution

Because the composition of air is given in mole percent, a basis of 1 g mol is chosen. The MW of the N_2 is not actually 28.0 but 28.2 because the value of the MW of the pseudo 79% N_2 is actually a combination of 78.084% N_2 and 0.934% Ar. The masses of the O_2 and pseudo N_2 are

Basis: 1 g mol of air

$$\text{Mass of } O_2 = \frac{1 \text{ g mol air}}{} \left| \frac{0.21 \text{ g mol } O_2}{\text{g mol air}} \right| \frac{32.00 \text{ g } O_2}{\text{g mol } O_2} = 6.72 \text{ g } O_2$$

$$\text{Mass of } N_2 = \frac{1 \text{ g mol air}}{} \left| \frac{0.79 \text{ g mol } N_2}{\text{g mol air}} \right| \frac{28.2 \text{ g } N_2}{\text{g mol } N_2} = 22.28 \text{ g } N_2$$

$$\text{Total} \qquad = 29.0 \text{ g air}$$

Example 2.12 Calculation of Average Molecular Weight

Since the discovery of superconductivity almost 100 years ago, scientists and engineers have speculated about how it can be used to improve the use of energy. Until recently most applications were not economically viable because the niobium alloys used had to be cooled below 23 K by liquid He. However, in 1987 superconductivity in Y-Ba-Cu-O material was achieved at 90 K, a situation that permits the use of inexpensive liquid N_2 cooling.

What is the molecular weight of the cell of a superconductor material shown in Figure E2.12? (The figure represents one cell of a larger structure.)

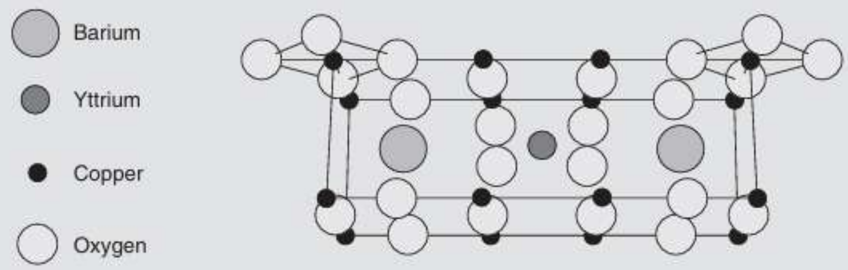

Figure E2.12

Solution

First look up the atomic weights of the elements from the table in Appendix B. Assume that one cell is a molecule. By counting the atoms you can find:

Element	Number of Atoms	Atomic Weight (g)	Mass (g)
Ba	2	137.34	2(137.34)
Cu	16	63.546	16(63.546)
O	37	16.00	37(16.00)
Y	1	88.905	1(88.905)
		Total	1972.3

The molecular weight of the cell is 1972.3 atomic masses/1 molecule or 1972.3 g/g mol. Check your calculations and check your answer to ensure that it is reasonable.

Mole fraction is simply the number of moles of a particular substance in a mixture or solution divided by the total number of moles present in the mixture or solution. This definition holds for gases, liquids, and solids. Similarly, the mass (weight) fraction is nothing more than the mass (weight) of the substance divided by the

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total mass (weight) of all of the substances present in the mixture or solution. Although mass fraction is the correct term, by custom ordinary engineering usage frequently employs the term weight fraction. These concepts can be expressed as

$$\text{mole fraction of A} = \frac{\text{moles of A}}{\text{total moles}}$$

$$\text{mass (weight) fraction of A} = \frac{\text{mass of A}}{\text{total mass}}$$

Example 2.13 Conversion between Mass (Weight) Fraction and Mole Fraction

An industrial-strength drain cleaner contains 5.00 kg of water and 5.00 kg of NaOH. What are the mass (weight) fraction and mole fraction of each component in the drain cleaner?

Solution

You are given the masses so it is easy to calculate the mass fractions. From these values you can then calculate the desired mole fractions.

A convenient way to carry out the calculations in such conversion problems is to form a table as shown below. Become skilled at doing so, because this type of problem and its inverse—that is, conversion of mole fraction to mass (weight) fraction—will occur more frequently than you would like. List the components, their masses, and their molecular weights in columns.

Basis: 10.0 kg of total solution

Component	kg	Weight Fraction	Mol. Wt.	kg mol	Mole Fraction
H_2O	5.00	$\frac{5.00}{10.0} = 0.500$	18.0	0.278	$\frac{0.278}{0.403} = 0.69$
NaOH	5.00	$\frac{5.00}{10.00} = 0.500$	40.0	0.125	$\frac{0.125}{0.403} = 0.31$
Total	10.00	1.000		0.403	1.00

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Example 2.14 Choosing a Basis

The dehydration of the lower-molecular-weight alkanes can be carried out using a ceric oxide (CeO) catalyst. What are the mass fraction and mole fraction of Ce and O in the catalyst?

Solution

Start the solution by selecting a basis. Because no specific amount of material is specified, the question "What do I have to start with?" does not help determine a basis. Neither does the question about the desired answer. Thus, selecting a convenient basis becomes the best choice. What do you know about CeO? You know from the formula that 1 mole of Ce is combined with 1 mole of O. Consequently, a basis of 1 kg mol (or 1 g mol, or 1 lb mol, etc.) would make sense. You can get the atomic weights for Ce and O from Appendix B, and then you are prepared to calculate the respective masses of Ce and O in CeO. The calculations for the mole and mass fractions for Ce and O in CeO are presented in the following table:

Basis: 1 kg mole of CeO

Component	kg mol	Mole Fraction	Mol. Wt.	kg	Mass Fraction
Ce	1	0.50	140.12	140.12	0.8975
O	1	0.50	16.0	16.0	0.1025
Total	2	1.00	156.12	156.12	1.0000

Example 2.15 Choosing a Basis (*Continued*)

Basis: 100 kg mol or lb mol of gas

Set up a table such as the following to make a compact presentation of the calculations. You do not have to, but making individual computations for each component is inefficient and more prone to errors.

Component	Percent = kg mol or lb mol	Mol. Wt.	kg or lb
CO_2	20.0	44.0	880
CO	30.0	28.0	840
CH_4	40.0	16.04	642
H_2	10.0	2.02	20
Total	100.0		2382

$$\text{Average molecular weight} = \frac{2382 \text{ kg}}{100 \text{ kg mol}} = 23.8 \text{ kg/kg mol}$$

Example 2.16 Changing Bases (*Continued*)

remove the SO_2, and adjust the basis for the calculations so that the gas becomes composed of only O_2 and N_2 with a percent composition totaling 100%:

Basis: 1.0 mol of gas

Components	Mol Fraction	Mol	Mol SO_2-Free	Mol Fraction SO_2-Free
O_2	0.20	0.20	0.20	0.20
N_2	0.78	0.78	0.78	0.80
SO_2	0.02	0.02		
	1.00	1.00	0.98	1.00

The round-off in the last column is appropriate given the original values for the mole fractions.

Density (we use the Greek symbol ρ) is the ratio of mass per unit volume such as kg/m^3 or lb/ft^3:

$$\rho = \text{density} = \frac{\text{mass}}{\text{volume}} = \frac{m}{V}$$

Specific volume (we use the symbol $\hat{V}$) is the inverse of density, such as cm^3/g or ft^3/lb:

$$\hat{V} = \text{specific volume} = \frac{\text{volume}}{\text{mass}} = \frac{V}{m}$$

Because density is the ratio of mass to volume, it can be used to calculate the mass given the volume or the volume knowing the mass. For example, given that the density of *n*-propyl alcohol is $0.804\ g/cm^3$, what would be the volume of 90.0 g of the alcohol? The calculation is

$$\frac{90.0g}{}\left|\frac{1\ cm^3}{0.804\ g}\right. = 112\ cm^3$$

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Example 2.17 Calculation of Density Given the Specific Gravity (*Continued*)

room temperature (22°C) and that the reference material is water at 4°C. Therefore, the reference density is 62.4 lb/ft^3 or 1.00×10^3 kg/m^3 (1.00 g/cm^3).

a. $$\frac{1.41\ \dfrac{\text{g P}}{\text{cm}^3}}{1.00\ \dfrac{\text{g H}_2\text{O}}{\text{cm}^3}} \left| \frac{1.00\ \dfrac{\text{g H}_2\text{O}}{\text{cm}^3}}{} \right. = 1.41\ \frac{\text{g P}}{\text{cm}^3}$$

b. $$\frac{1.41\ \dfrac{\text{lb}_m\text{ P}}{\text{ft}^3}}{1.00\ \dfrac{\text{lb}_m\text{ H}_2\text{O}}{\text{ft}^3}} \left| \frac{62.4\ \dfrac{\text{lb}_m\text{H}_2\text{O}}{\text{ft}^3}}{} \right. = 88.0\ \frac{\text{lb}_m\text{ P}}{\text{ft}^3}$$

c. $$\frac{1.41\text{ g P}}{\text{cm}^3}\left|\left(\frac{100\text{ cm}}{1\text{ m}}\right)^3\right|\frac{1\text{ kg}}{1000\text{ g}} = 1.41 \times 10^3\ \frac{\text{kg P}}{\text{m}^3}$$

You should become acquainted with the fact that in the petroleum industry the specific gravity of petroleum products is often reported in terms of a hydrometer scale called **°API**. The equations that relate the API scale to density and vice versa are

$$°\text{API} = \frac{141.5}{\text{sp. gr.}\ \dfrac{60°\text{F}}{60°\text{F}}} - 131.5 \qquad \text{(API gravity)} \qquad (2.4)$$

or

$$\text{sp.gr.}\ \frac{60°}{60°} = \frac{141.5}{°\text{API} + 131.5} \qquad (2.5)$$

The volume and therefore the density of petroleum products vary with temperature, and the petroleum industry has established 60°F as the standard temperature for specific gravity and API gravity. The CD in the back of the book contains data for petroleum products.

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Example 2.18 Application of Specific Gravity to Calculate Mass and Moles

In the production of a drug having a molecular weight of 192, the exit stream from the reactor containing water and the drug flows at the rate of 10.5 L/min. The drug concentration is 41.2% (in water), and the specific gravity of the solution is 1.024. Calculate the concentration of the drug (in kilograms per liter) in the exit stream, and the flow rate of the drug in kilogram moles per minute.

Solution

Read the problem carefully because this example is more complicated than the previous examples. You have a problem with some known properties including specific gravity. The strategy for the solution is to use the specific gravity to get the density, from which you can calculate the moles per unit volume.

For the first part of the problem, you want to transform the mass fraction of 0.412 into mass per liter of the drug. Take 1.000 kg of the exit solution as a basis because the mass fraction of the drug in the product is specified in the problem statement. Figure E2.18 shows the output.

Basis: 1.000 kg solution

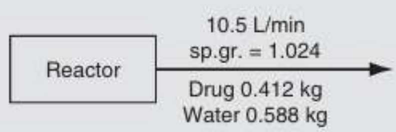

Figure E2.18

How do you get mass of drug per volume of solution (the density) from the given data, which are in terms of the fraction of the drug (0.412)? Use the given specific gravity of the solution. Calculate the density of the solution as follows:

$$\text{density of solution} = (\text{sp.gr.})(\text{density of reference})$$

$$\text{density of solution} = \frac{1.024\,\dfrac{\text{g soln}}{\text{cm}^3\text{ soln}}}{1.000\,\dfrac{\text{g H}_2\text{O}}{\text{cm}^3\text{ H}_2\text{O}}}\left|\frac{1.000\,\dfrac{\text{g H}_2\text{O}}{\text{cm}^3\text{ H}_2\text{O}}}{}\right. = 1.024\,\frac{\text{g soln}}{\text{cm}^3\text{ soln}}$$

The detail of the calculation of the density of the solution showing the units may seem excessive but is presented to make the calculation clear.

Next, convert the amount of drug in 1.000 kg of solution to mass of drug per volume of solution using the density previously calculated, recognizing that there is 0.412 kg of the drug for the basis of 1.000 kg of solution.

$$\frac{0.412\text{ kg drug}}{1.000\text{ kg soln}}\left|\frac{1.0254\text{ g soln}}{1\text{ cm}^3\text{ soln}}\right|\frac{1\text{ kg soln}}{10^3\text{ g soln}}\left|\frac{1000\text{ cm}^3\text{ soln}}{1\text{ L soln}}\right. = 0.422\text{ kg drug/L soln}$$

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Example 2.18 Application of Specific Gravity to Calculate Mass and Moles (*Continued*)

Note that a distinction is drawn between properties of the solution (e.g., g soln, L soln) and the mass of the drug to prevent confusion in the cancellation of units.

To get the flow rate, take a different basis, namely, 1 min.

Basis: 1 min = 10.5 L of solution

Convert the selected volume to mass and then to moles using the information previously calculated:

$$\frac{10.5\text{ L soln}}{1\text{ min}}\left|\frac{0.422\text{ kg drug}}{1\text{ L soln}}\right|\frac{1\text{ kg mol drug}}{192\text{ kg drug}} = 0.0231\text{ kg mol/min}$$

Concentration designates the amount of a component (solute) in a mixture divided by the total of the mixture. The amount of the component of interest is usually expressed in terms of the mass or moles of the component, whereas the amount of the mixture can be expressed as the corresponding volume or mass of the mixture. Some common examples that you will encounter are:

- **Mass per unit volume** such as lb_m of solute/ft^3 of solution, g of solute/L, lb_m of solute/bbl, kg of solute/m^3.
- **Moles per unit volume** such as lb mol of solute/ft^3 of solution, g mol of solute/L, g mol of solute/cm^3.
- **Mass (weight) fraction**—the ratio of the mass of a component to the total mass of the mixture, a fraction (or a percent).
- **Mole fraction**—the ratio of the moles of a component to the total moles of the mixture, a fraction (or a percent).
- **Parts per million (ppm) and parts per billion (ppb)**—a method of expressing the concentration of extremely dilute solutions; ppm is equivalent to a mass (weight) ratio for solids and liquids. It is a mole ratio for gases.
- **Parts per million by volume (ppmv) and parts per billion by volume (ppbv)**—the ratio of the volume of the solute per volume of the mixture (usually used only for gases).

Example 2.19 Nitrogen Requirements for the Growth of Cells

In normal living cells, the nitrogen requirement for the cells is provided from protein metabolism (i.e., consumption of protein in the cells). When cells are grown commercially such as in the pharmaceutical industry, $(NH_4)_2SO_4$ is usually used as the source of nitrogen. Determine the amount of $(NH_4)_2SO_4$ consumed in a fermentation medium in which the final cell concentration is 35 g/L in a 500 L volume of fermentation medium. Assume that the cells contain 9 wt % N, and that $(NH_4)_2SO_4$ is the only nitrogen source.

Solution

Basis: 500 L of solution containing 35 g/L

$$\frac{500\text{ L}}{}\left|\frac{35\text{ g cell}}{\text{L}}\right|\frac{0.09\text{ g N}}{\text{g cell}}\left|\frac{\text{g mol}}{14\text{ g N}}\right|\frac{1\text{ g mol }(NH_4)_2SO_4}{2\text{ g mol N}}\Bigg|$$

$$\frac{132\text{ g }(NH_4)_2SO_4}{\text{g mol }(NH_4)_2SO_4} = 7425\text{ g }(NH_4)_2SO_4$$

Here is a list of typical measures of concentration given in the set of guidelines by which the Environmental Protection Agency defines the extreme levels at which the five most common air pollutants could harm people if they are exposed to these levels for the stated periods of exposure:

1. **Sulfur dioxide:** 365 $\mu g/m^3$ averaged over a 24 hr period
2. **Particulate matter** (10 μm or smaller): 150 $\mu g/m^3$ averaged over a 24 hr period
3. **Carbon monoxide:** 10 mg/m^3 (9 ppm) when averaged over an 8 hr period; 40 mg/m^3 (35 ppm) when averaged over 1 hr
4. **Nitrogen dioxide:** 100 $\mu g/m^3$ averaged over 1 yr
5. **Ozone:** 0.12 ppm measured over 1 hr

Note that the gas concentrations are mostly mass/volume except for the ppm.

Example 2.20 Use of ppm

The current OSHA 8 hr limit for HCN in air is 10.0 ppm. A lethal dose of HCN in air is (from the *Merck Index*) 300 mg/kg of air at room temperature. How many milligrams of HCN per kilogram of air is 10.0 ppm? What fraction of the lethal dose is 10.0 ppm?

Solution

In this problem you have to convert ppm in a gas (a mole ratio, remember!) to a mass ratio.

Basis: 1 kg of the air-HCN mixture

We can treat the 10.0 ppm as 10.0 g mol HCN/10^6 g mol air because the amount of HCN is so small when added to the air in the denominator of the ratio.

The 10.0 ppm is

$$\frac{10.0 \text{ g mol HCN}}{10^6(\text{air} + \text{HCN})\text{g mol}} = \frac{10.0 \text{ g mol HCN}}{10^6 \text{ g mol air}}$$

(*Continues*)

Example 2.20 Use of ppm (*Continued*)

Next, get the MW of HCN so that it can be used to convert moles of HCN to mass of HCN; the MW = 27.03. Then

$$\frac{10.0 \text{ g mol HCN}}{10^6 \text{ g mol air}}\left|\frac{27.03 \text{ g HCN}}{1 \text{ g mol HCN}}\right|\frac{1 \text{ g mol air}}{29 \text{ g air}}\left|\frac{1000 \text{ mg HCN}}{1 \text{ g HCN}}\right|\frac{1000 \text{ g air}}{1 \text{ kg air}}$$

$$= 9.32 \text{ mg HCN/kg air}$$

$$\frac{9.32}{300} = 0.031$$