1.2Moles, Density and Concentration

1.2.1 Mole

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

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

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For example

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

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

- **The atomic weight** of an element is the mass of an atom based on the scale that assigns a mass of exactly 12 to the carbon isotope ^{12}C.
- A **compound** is composed of more than one atom, and the molecular weight of the compound is nothing more than the sum of the weights of atoms of which it is composed.

Example 1

What is the molecular weight of the following cell of a superconductor material? (The figure represents one cell of a larger structure.)

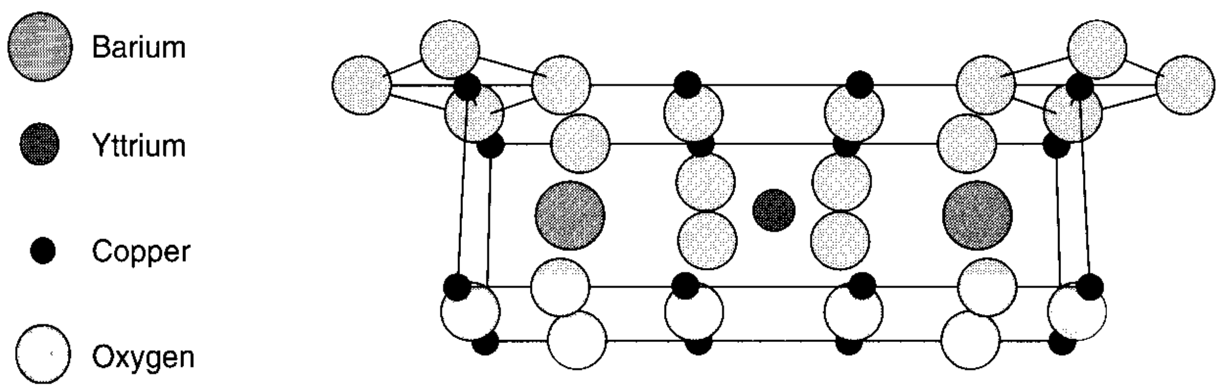

Figure E2.1

Solution

Element	Number of atoms	Atomic weights	Mass (g)
Ba	2	137.34	2(137.34)
Cu	16	63.546	16(63.546)
O	24	16.00	24(16.00)
Y	1	88.905	1(88.905)
		Total	1764.3

The molecular weight of the cell is 1764.3 g/g mol.

Example 2:

If a bucket holds 2.00 lb of NaOH (MW=40), how many
a) Pound moles of NaOH does it contain?

b) Gram moles of NaOH does it contain?

Solution

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

$$\textbf{(b}_1\textbf{)}\quad \frac{2.00\text{ lb NaOH}}{}\left|\frac{1\text{ lb mol NaOH}}{40.0\text{ lb NaOH}}\right|\frac{454\text{ g mol}}{1\text{ lb mol}} = 22.7\text{ g mol}$$

$$\textbf{(b}_2\textbf{)}\quad \frac{2.00\text{ lb NaOH}}{}\left|\frac{454\text{ g}}{1\text{ lb}}\right|\frac{1\text{ g mol NaOH}}{40.0\text{ g NaOH}} = 22.7\text{ g mol}$$

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Example 3:

How many pounds of NaOH (MW=40) are in 7.50 g mol of NaOH?

Solution

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

1.2.2 Density

Density is the ratio of mass per unit volume, as for example, kg/m^3 or lb/ft^3. Density has both a numerical value and units. Specific volume is the inverse of density, such as cm^3/g or ft^3/lb.

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

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

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

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

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❖ In a packed bed of solid particles containing void spaces, the bulk density is

$$\rho_B = \text{bulk density} = \frac{\text{total mass of solids}}{\text{total empty bed volume}}$$

❖ A homogeneous mixture of two or more components, whether solid, liquid, or gaseous, is called a solution. For some solutions, the density of the solution is

$$V = \sum_{i=1}^{n} V_i \qquad \text{where } n = \text{number of components}$$

$$m = \sum_{i=1}^{n} m_i$$

$$\rho_{\text{solution}} = \frac{m}{V}$$

For others you cannot.

Specific Gravity

Specific gravity: is commonly thought of as a dimensionless ratio.

$$\text{sp.gr. of } A = \textbf{specific gravity} \text{ of } A = \frac{(\text{g/cm}^3)_A}{(\text{g/cm}^3)_{ref}} = \frac{(\text{kg/m}^3)_A}{(\text{kg/m}^3)_{ref}} = \frac{(\text{lb/ft}^3)_A}{(\text{lb/ft}^3)_{ref}}$$

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♦ The reference substance for **liquids** and **solids** normally is **water.**

♦ The density of water is **1.000 g/cm³**, **1000 kg/m³**, or **62.43 lb/ft³ at 4°C.**

♦ The specific gravity of **gases** frequently is referred to **air**, but may be referred to other gases.

For Example If dibromopentane (DBP) has a specific gravity of 1.57, what is the density in (a) g/cm³? (b) lbm/ft³? and
(c) kg/m³?

$$\textbf{(a)}\quad \frac{1.57\,\dfrac{\text{g DBP}}{\text{cm}^3}}{1.00\,\dfrac{\text{g H}_2\text{O}}{\text{cm}^3}}\left|\,\frac{1.00\,\dfrac{\text{g H}_2\text{O}}{\text{cm}^3}}{}\right. = 1.57\,\frac{\text{g DBP}}{\text{cm}^3}$$

$$\textbf{(b)}\quad \frac{1.57\,\dfrac{\text{lb DBP}}{\text{ft}^3}}{1.00\,\dfrac{\text{lb H}_2\text{O}}{\text{ft}^3}}\left|\,\frac{62.4\,\dfrac{\text{lb H}_2\text{O}}{\text{ft}^3}}{}\right. = 97.97\,\frac{\text{lb DBP}}{\text{ft}^3}$$

$$\textbf{(c)}\quad \frac{1.57\text{g DBP}}{\text{cm}^3}\left|\left(\frac{100\text{ cm}}{1\text{ m}}\right)^3\right|\frac{1\text{ kg}}{1000\text{ g}} = 1.57\times 10^3\,\frac{\text{kg DBP}}{\text{m}^3}$$

or

$$\frac{1.57\,\dfrac{\text{kg DBP}}{\text{m}^3}}{1.00\,\dfrac{\text{kg H}_2\text{O}}{\text{m}^3}}\left|\,\frac{\dfrac{1.00\times 10^3\text{kg H}_2\text{O}}{\text{m}^3}}{}\right. = 1.57\times 10^3\,\frac{\text{kg DBP}}{\text{m}^3}$$

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Example 4

If a 70% (by weight) solution of glycerol has a specific gravity of 1.184 at 15°C, what is the density of the solution in (a) g/cm^3? (b) lbm/ft^3? and (c) kg/m^3?

Solution

(a) (1.184 g glycerol/ cm^3)/(1 g water/ cm^3) * (1 g water/ cm^3) = 1.184 g solution/cm^3.

(b) (1.184 lb glycerol/ft^3)/(1 lb water/ft^3) * (62.4 lb water/ft3) = 73.9 lb solution/ft^3.

(c) (1.184 kg glycerol/m^3)/(1 kg water/m^3) * (1000 kg water/m^3) = 1.184 * l03 kg solution/m^3

The specific gravity of petroleum products is often reported in terms of a hydrometer scale called °API. The equation for the API scale is

$$°API = \frac{141.5}{sp.gr.\frac{60°F}{60°F}} - 131.5 \qquad (\text{API gravity}) \tag{2.1}$$

or

$$sp.gr.\frac{60°}{60°} = \frac{141.5}{°API + 131.5} \tag{2.2}$$

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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 volume and API gravity.

Example 5:

In the production of a drug having a molecular weight of 192, the exit stream from the reactor flows at a 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 kg/L) in the exit stream, and the flow rate of the drug in kg mol/min.

Solution

Take 1 kg of the exit solution as a basis for convenience.

Basis: 1 kg solution

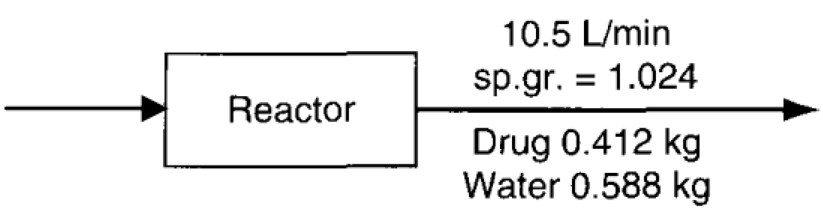

Figure E2.5

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

$$\frac{0.412\text{ kg drug}}{1.000\text{ kg soln}}\left|\frac{1.024\text{ g soln}}{1\text{ cm}^3}\right|\frac{1\text{ kg}}{10^3\text{ g}}\left|\frac{10^3\text{cm}^3}{1\text{ L}}\right. = 0.422\text{ kg drug/L soln}$$

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

Basis: 1 min = 10.5 L solution

$$\frac{10.5 \text{ L soln}}{1 \text{ min}} \left| \frac{0.422 \text{ kg drug}}{1 \text{ L soln}} \right| \frac{1 \text{ kg mol drug}}{192 \text{ kg drug}} = 0.023 \text{ kg mol/min}$$

Flow Rate

For continuous processes the flow rate of a process stream is the rate at which material is transported through a pipe. The mass flow rate (m) of a process stream is the mass (m) transported through a line per unit time (t).

$$\dot{m} = \frac{m}{t}$$

The volumetric flow rate (F) of a process stream is the volume (V) transported through a line per unit time.

$$F = \frac{V}{t}$$

The molar flow (n) rate of a process stream is the number of moles (n) of a substance transported through a line per unit time.

$$\dot{n} = \frac{n}{t}$$

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Mole Fraction and Mass (Weight) Fraction

- Mole fraction is simply the number of moles of a particular compound in a mixture or solution divided by the total number of moles 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 compound divided by the total mass (weight) of all of the compounds in the mixture or solution.

Mathematically, these ideas can be expressed as

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

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

Mole percent and **mass (weight)** percent are the respective fractions times **100.**

Example 6:

An industrial-strength drain cleaner contains 5 kg of water and 5 kg of NaOH.

What are the mass (weight) fractions and

mole fractions of each component in the drain cleaner container?

Solution

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Basis: 10 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

The kilogram moles are calculated as follows:

$$\frac{5.00 \text{ kg } H_2O}{} \left| \frac{1 \text{ kg mol } H_2O}{18.0 \text{ kg } H_2O} \right. = 0.278 \text{ kg mol } H_2O$$

$$\frac{5.00 \text{ kg NaOH}}{} \left| \frac{1 \text{ kg mol NaOH}}{40.0 \text{ kg NaOH}} \right. = 0.125 \text{ kg mol NaOH}$$

Adding these quantities together gives the total kilogram moles.

Example 7:

In normal living cells, the nitrogen requirement for the cells is provided from protein metabolism (i.e., consumption of the protein in the cells). When individual cells are commercially grown, $(NH_4)_2SO_4$ 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 the 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 solution containing 35 g/L

$$\frac{500\ \text{L}}{}\left|\frac{35\ \text{g cell}}{\text{L}}\right|\frac{0.09\ \text{g N}}{1\ \text{g cell}}\left|\frac{1\ \text{g mol N}}{14\ \text{g N}}\right. \times \frac{1\ \text{g mol}\ (NH_4)_2SO_4}{1\ \text{g mol N}}\left|\frac{132\ \text{g}\ (NH_4)_2SO_4}{1\ \text{g mol}\ (NH_4)_2SO_4}\right. = 14{,}850\ \text{g}\ (NH_4)_2SO_4$$

Analyses of Multi Components Solutions and Mixtures

The composition of gases will always be presumed to be given in **mole percent** or **fraction** unless specifically stated otherwise.

The **composition** of **liquids and solids** will be given by **mass (weight) percent** or fraction unless otherwise
specifically stated.

For Example Table below lists the detailed composition of dry air (composition of air 21% O_2 and 79% N_2).

Basis 100 mol of air

Component	Moles = percent	Mol. wt.	Lb or kg	Weight %
O_2	21.0	32	672	23.17
N_2	79.0	28.2	2228	76.83
Total	100		2900	100.00

The average molecular weight is 2900 lb/100 lb mol = 29.0, or 2900 kg/100 kg mol = 29

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1.2.3 Concentration

Concentration generally refers to the quantity of some substance per unit volume.

a. Mass per unit volume (lb of solute/ft^3 of solution, g of solute/L, lb of solute/barrel, kg of solute/m^3).

b. Moles per unit volume (lb mol of solute/ft^3 of solution, g mol of solute/L, g mol of solute/cm^3).

c. Parts per million (ppm); parts per billion (ppb), a method of expressing the concentration of extremely dilute solutions; ppm is equivalent to a mass (weight) fraction for solids and liquids because the total amount of material is of a much higher order of magnitude than the amount of solute; it is a mole fraction for gases.

d. Parts per million by volume (ppmv) and parts per billion by volume (ppbv)

e. Other methods of expressing concentration with which you may be familiar are molarity (g mol/L), molality (mole solute/kg solvent), and normalit (equivalents/L).

Example 8:

The current OSHA 8-hour limit for HCN (MW = 27.03) 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 mg HCN/kg air is 10.0 ppm? What fraction of the lethal dose is 10.0 ppm?

Solution

Basis: 1 kg mol of the air/HCN mixture

The 10.0 ppm is $\dfrac{10.0 \text{ g mol HCN}}{10^6(\text{air} + \text{HCN})\text{g mol}} = \dfrac{10.0 \text{ g mol HCN}}{10^6 \text{ g mol air}}$

a. $\dfrac{10.0 \text{ g mol HCN}}{10^6 \text{ g mol air}} \Bigg| \dfrac{27.03 \text{ g HCN}}{1 \text{ g mol HCN}} \Bigg| \dfrac{1 \text{ g mol air}}{29 \text{ g air}} \Bigg| \dfrac{1000 \text{ mg HCN}}{1 \text{ g HCN}} \times \dfrac{1000 \text{ g air}}{1 \text{ kg air}} = 9.32 \text{ mg HCN/kg air}$

b. $\dfrac{9.32}{300} = 0.031$

Example 9:

A solution of HNO_3 in water has a specific gravity of 1.10 at 25°C. The concentration of the HNO_3 is 15 g/L of
solution. What is the

a. Mole fraction of HNO_3 in the solution?

b. ppm of HNO3 in the solution?

Solution

Basis: 1 L of solution

$$\frac{15 \text{ g } HNO_3}{1 \text{ L soln}} \Bigg| \frac{1 \text{ L}}{1000 \text{ cm}^3} \Bigg| \frac{1 \text{ cm}^3}{1.10 \text{ g soln}} = 0.01364 \frac{\text{g } HNO_3}{\text{g soln}}$$

Basis: 100 g solution

The mass of water in the solution is: 100 - 0.0134 = 99.986 g H_2O.

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		g	MW	g mol	mol fraction
a.	HNO_3	0.01364	63.02	2.164×10^{-4}	3.90×10^{-5}
	H_2O	99.986	18.016	5.550	1.00
	Total			5.550	1.00

b. $$\frac{0.01364}{1} = \frac{13{,}640}{10^6} \text{ or } 13{,}640 \text{ ppm}$$

Example 10:

To avoid the possibility of explosion in a vessel containing gas having the composition of 40% N_2, 45% O_2, and 15% CH_4, the recommendation is to dilute the gas mixture by adding an equal amount of pure N_2. What is the final mole fraction of each gas?

Solution

The basis is 100 moles of initial gas

Composition	*Original Mixture mol%*	*After Addition N_2*	**Final Mixture Mole Fraction**
N_2	40 ➡ + 100	140	140/200 = 0.70
O_2	45	45	45/200 = 0.23
CH_4	15	15	15/200 = 0.07
Total	100	200	1.00

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H.w: Questions

1. Answer the following questions true or false:

a. The pound mole is comprised of 2.73 x 1026 molecules

b. The kilogram mole is comprised of 6.022 x 1026 molecules.

c. Molecular weight is the mass of a compound or element per mole.

2. What is the molecular weight of acetic acid (CH_3COOH)?

3. For numbers such as 2 mL of water + 2 mL of ethanol, does the sum equal to 4 mL of the solution?

4. Answer the following questions true or false:

a. The inverse of the density is the specific volume.

b. Density of a substance is the mass per unit volume.

c. The density of water is less than the density of mercury.

5. A cubic centimeter of mercury has a mass of 13.6 g at Earth's surface. What is the density of mercury?

6. What is the approximate density of water at room temperature in kg/m3?

7. For liquid HCN, a handbook gives: sp. gr. 10°C/4°C = 1.2675. What does this statement mean?

8. Answer the following questions true or false:

a. The density and specific gravity of mercury are the same.

b. Specific gravity is the ratio of two densities.

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c. If you are given the value of a reference density, you can determine the density of a substance of interest by multiplying by the specific gravity.

d. The specific gravity is a dimensionless quantity.

9. A mixture is reported as 15% water and 85% ethanol. Should the percentages be deemed to be by mass, mole, or volume?

10. Answer the following questions true or false:

a) In engineering practice the compositions of liquids and solids are usually denoted in weight (mass)

fraction or percent.

b) In engineering practice the composition of gases is usually denoted in mole fraction or percent.

c) e. A pseudo-average molecular weight can be calculated for a mixture of pure components whether

solid, liquid, or gases.

11. Do parts per million denote a concentration that is a mole ratio?

12. Does the concentration of a component in a mixture depend on the amount of the mixture?

13. Pick the correct answer. How many ppm are there in 1 ppb? (a) 1000, (b) 100, (c) 1, (d) 0.1, (e) 0.01, (f) 0.001?

14. How many ppb are there in 1 ppm?

15. Does 50 ppm represent an increase of five times a value of 10 ppm?