Chemical Calculations

References : 1. General Chemistry- principles and modern applications (Petrucci, Herring, Madura, Bissonnette)
2. Chemistry 10th Edition (Raymond Chang)

Measurement of Matter: SI (Metric) Units

Chemistry is a *quantitative science, which means that in many cases we can* measure a property of a substance and compare it with a standard having a known value of the property.

The scientific system of measurement is called the *Système Internationale d Unités (International System of Units) and is abbreviated* ***SI.***

SI Base Quantity

Physical quantity	Unit
Length	metre, m
Mass	kilogram, kg
Time	second, s
Temperature	kelvin, K
Amount of substance	mole, mol
Electric current	ampere, A
Luminous intensity	candela, cd

TABLE 1.2 SI Prefixes

Multiple	Prefix
10^{18}	exa (E)
10^{15}	peta (P)
10^{12}	tera (T)
10^{9}	giga (G)
10^{6}	mega (M)
10^{3}	kilo (k)
10^{2}	hecto (h)
10^{1}	deka (da)
10^{-1}	deci (d)
10^{-2}	centi (c)
10^{-3}	milli (m)
10^{-6}	micro (μ)[a]
10^{-9}	nano (n)
10^{-12}	pico (p)
10^{-15}	femto (f)
10^{-18}	atto (a)
10^{-21}	zepto (z)
10^{-24}	yocto (y)

[a]The Greek letter μ (pronounced "mew").

- Most measurements in chemistry are made in SI units. Sometimes we must convert between SI units, as when converting kilometers to meters.
- At other times we must convert measurements expressed in non-SI units into SI units, or from SI units into non-SI units.
- In all of these cases we can use a *conversion factor or a series of conversion factors in a scheme called a conversion pathway.*

To go from one unit to another, we need a conversion factor.

We need 3 important pieces of information:

- Desired amount and units
- Initial amount and units
- Conversion factor

The general form of a unit conversion calculation is:

(desired amount)= (initial amount) x (conversion factor)

Mass

- **Mass** describes the quantity of matter in an object. In SI the standard of mass is 1 kilogram (kg), which is a fairly large unit for most applications in chemistry. More commonly we use the unit gram (g) (about the mass of three aspirin tablets).
- **Weight** is the force of gravity on an object. It is directly proportional to mass, as shown in the following mathematical expressions.

$$W \propto m \text{ and } W = g \times m$$

An object has a fixed mass (m), which is independent of where or how the mass is measured. Its weight (W), however, may vary because the acceleration due to gravity (g) varies slightly from one point on Earth to another.

Density

Density is the ratio of mass to volume.

$$\text{density } (d) = \frac{\text{mass } (m)}{\text{volume } (V)}$$

Mass and volume are both extensive properties.

An **extensive property is** *dependent on the quantity of matter observed. However, if we divide the mass* of a substance by its volume, we obtain density, an intensive property.

An **intensive property** is *independent of the amount of matter observed*. ***Thus, the*** density of pure water at 25 °C has a unique value, whether the sample fills a small beaker (small mass/small volume) or a swimming pool (large mass/large volume).

Intensive properties are especially useful in chemical studies because they can often be used to identify substances.

The SI base units of mass and volume are kilograms and cubic meters, respectively, but chemists generally express mass in grams and volume in cubic centimeters or milliliters. Thus, the most commonly encountered density unit is grams per cubic centimeter (g/cm^3) or the identical unit grams per milliliter (g/mL).

The Concept of the Mole and the Avogadro Constant

- The SI quantity that describes an amount of substance by relating it to a number of particles of that substance is called the mole (abbreviated mol).
- A mole is the amount of a substance that contains the same number of elementary entities as there are atoms in exactly 12 g of pure carbon-12.
- This definition carefully avoids saying that the entities to be counted are always atoms. As a result, we can apply the concept of a mole to any quantity that we can represent by a symbol or formula—atoms, ions, formula units, or molecules.
- The “number of elementary entities (atoms, molecules, and so on)” in a mole is the Avogadro constant, N_A .

$$\boxed{N_A = 6.022140857 \times 10^{23}\ \text{mol}^{-1}}$$

Composition of Chemical Compounds

- A chemical formula conveys considerable quantitative information about a compound and its constituent elements. We have already learned how to determine the molar mass of a compound, and, in this section, we consider some other types of calculations based on the chemical formula.
- The colorless, volatile liquid halothane has been used as a fire extinguisher and also as an inhalation anesthetic. Both its empirical and molecular formulas are $C_2HBrClF_3$,its molecular mass is 197.38 u, and its molar mass is as calculated below:

$$\begin{aligned} M_{C_2HBrClF_3} &= 2M_C + M_H + M_{Br} + M_{Cl} + 3M_F \\ &= [(2 \times 12.011) + 1.008 + 79.904 + 35.45 + (3 \times 18.9984)]\ g/mol \\ &= 197.38\ g/mol \end{aligned}$$

The molecular formula of $C_2HBrClF_3$ tells us that per mole of halothane there are two moles of C atoms, one mole each of H, Br, and Cl atoms, and three moles of F atoms. This factual statement can be turned into conversion factors to answer such questions as, “How many C atoms are present per mole of halothane?” In this case, the factor needed is 2 mol/ mol $C_2HBrClF_3$. That is,

$$
\begin{aligned}
?\ \text{C atoms} &= 1.000 \text{ mol } C_2HBrClF_3 \times \frac{2 \text{ mol C}}{1 \text{ mol } C_2HBrClF_3} \times \frac{6.022 \times 10^{23} \text{ C atoms}}{1 \text{ mol C}} \\
&= 1.204 \times 10^{24} \text{ C atoms}
\end{aligned}
$$

Calculating Percent Composition from a Chemical Formula

When chemists believe that they have synthesized a new compound, a sample is generally sent to an analytical laboratory where its percent composition is determined. This experimentally determined percent composition is then compared with the percent composition calculated from the formula of the expected compound. In this way, chemists can see if the compound obtained could be the one expected.

- Equation (3.1) establishes how the mass percent of an element in a compound is calculated. In applying the equation, think in terms of the following steps.

1. **Determine the molar mass of the compound.** This is the *denominator* in equation (3.1).
2. **Determine the contribution of the given element to the molar mass.** This product of the formula subscript and the molar mass of the element appears in the *numerator* of equation (3.1).
3. **Formulate the ratio of the mass of the given element to the mass of the compound as a whole.** This is the ratio of the numerator from step 2 to the denominator from step 1.
4. **Multiply this ratio by 100% to obtain the mass percent of the element.**

$$\text{mass \% element} = \frac{\begin{pmatrix}\text{number of}\\ \text{atoms of element}\\ \text{per formula unit}\end{pmatrix} \times \begin{pmatrix}\text{molar mass}\\ \text{of element}\end{pmatrix}}{\text{molar mass of compound}} \times 100\% \qquad \textbf{(3.1)}$$

Establishing Formulas from the Experimentally Determined Percent Composition of Compounds

- At times, a chemist isolates a chemical compound—say, from an exotic tropical plant—and has no idea what it is. A report from an analytical laboratory on the percent composition of the compound yields data needed to determine its formula.
- Percent composition establishes the relative proportions of the elements in a compound on a mass basis. A chemical formula requires these proportions to be on a mole basis, that is, in terms of numbers of atoms.