Chapter 8
How to Do Chemical Calculations

Chemistry is both a qualitative and a quantitative science. In the laboratory, it is important to be able to measure quantities of chemical substances and, as was introduced in Chapter 4, Section 4.4, the key to measuring quantities of chemicals is the mole.

8.1 Background

In Chapter 1, Section 1.3, it was described how, even in this century, many important pharmaceuticals are derived from plant and animal sources. When an extract of a plant or specific animal organ is found to have an effect on the progress of a disease, then it is vital to discover which particular chemical compound is the cause of the beneficial effect. After that compound has been separated, the next step is to identify the arrangement of the atoms in the compound (the chemical structure). When that has been accomplished, the compound can be synthesized in the laboratory for mass production. Also, knowing the chemical structure enables chemists to synthesize compounds with slightly different arrangements of atoms which may be more effective and/or may have fewer side effects. This Chapter will introduce calculations that show how chemical formulas of such compounds can be derived from experimental measurements.

Figure 8.1 (left) The rosy periwinkle plant found in the island country of Madagascar is the source of (right) an important anti-cancer drug, vinblastine

8.2 Mass Measurements for Compounds

Chapter 4, Section 4.3 introduced the concept of atomic mass while Section 4.5 discussed molar mass. Just as calculations are possible for elements and atoms of elements, so there are parallel calculations for compounds but with an additional step in the calculation.

FORMULA AND MOLECULAR MASS

One complication is that there are, as was shown in Chapter 6, two types of chemical compounds: those in which outer electrons are transferred from one atom to the other (ionic compounds) and those in which atoms share electrons (covalent compounds). A different term is used for each type of compound.

For an ionic compound, the term 'formula mass' is used:
The ***formula mass*** is the mass of one formula unit of a compound.
For a covalent compound, the term 'molecular mass' is used:
The ***molecular mass*** is the mass of one molecule of a compound.

In Chapter 4, Section 4.3, the mass of one atom of an element was found from the average atomic mass value in the Periodic Table. To do likewise for a compound, the same procedure is followed except it is necessary to sum the masses of the individual atoms, taking into account the number of each atom in that compound.

EXAMPLE 8.1

Calculate the formula mass of potassium chloride, KCl.

Answer

From the Periodic Table, the atomic mass of potassium is 39.1 u and that of chlorine is 35.5 u.
There is one ion of each element in the formula unit.
The formula mass of KCl = $(1 \times 39.1 \text{ u}) + (1 \times 35.5 \text{ u}) = 74.6$ u

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EXAMPLE 8.2

Calculate the molecular mass of sulfur dioxide, SO_2.

Answer

From the Periodic Table, the atomic mass of sulfur is 32.1 u and that of oxygen is 16.0 u.
There is one atom of sulfur and two atoms of oxygen in each molecule.
The molecular mass of $SO_2 = (1 \times 32.1 \text{ u}) + (2 \times 16.0 \text{ u}) = 64.1$ u

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MOLAR MASS

Though it is sometimes useful to be able to calculate the mass of a formula unit or molecule, it is much more useful to calculate the mass of a mole of formula units or a mole of molecules. For this purpose, the term 'molar mass' is used.
The ***molar mass*** is the mass of one mole of any compound.

EXAMPLE 8.3

Calculate the molar mass of sodium phosphate, Na_3PO_4.

Answer

From the Periodic Table, the molar mass of sodium is 23.0 g; of phosphorus, 31.0 g; and of oxygen, 16.0 g.

The molar mass of $Na_3PO_4 = (3 \times 23.0 \text{ g}) + (1 \times 31.0 \text{ g}) + (4 \times 16.0 \text{ g}) = 164.0 \text{ g·mol}^{-1}$

8.3 Mole Calculations for Compounds

In Chapter 4, Section 4.4, it was shown how it is possible to interconvert mass, moles, and number of atoms for elements. Here the similar calculations for compounds will be introduced.

INTERCONVERSION OF MASS AND MOLES

With compounds, the same procedure is followed, except the molar mass of the compound has to be determined first.

EXAMPLE 8.4

A mass of 10.7 g of calcium iodide, CaI_2, corresponds to how many moles of compound?

Answer

First, calculate the molar mass of $CaI_2 = (1 \times 40.1 \text{ g}) + (2 \times 126.9 \text{ g}) = 293.9 \text{ g·mol}^{-1}$

Strategy	Relationship
mass $CaI_2 \rightarrow$ mol CaI_2	$1 \text{ mol} \equiv 293.9 \text{ g } CaI_2$

$$\text{Mol of CaI}_2 = 10.7 \text{ g} \times \left(\frac{1 \text{ mol}}{293.9 \text{ g}}\right) = 3.64 \times 10^{-2} \text{ mol CaI}_2$$

EXAMPLE 8.5

What is the mass of 1.40 mol of ammonium sulfate, $(NH_4)_2SO_4$?

Answer

First, calculate the molar mass of $(NH_4)_2SO_4$
$$= (2 \times 14.0 \text{ g}) + (8 \times 1.01 \text{ g}) + (1 \times 32.1 \text{ g}) + (4 \times 16.0 \text{ g}) = 132.1 \text{ g·mol}^{-1}$$

Strategy	Relationship
Mol of $(NH_4)_2SO_4 \rightarrow$ mass $(NH_4)_2SO_4$	$1 \text{ mol} \equiv 132.1 \text{ g } (NH_4)_2SO_4$

$$\text{Mass of (NH}_4)_2\text{SO}_4 = 1.40 \text{ mol} \times \left(\frac{132.1 \text{ g}}{1 \text{ mol}}\right) = 185 \text{ g (NH}_4)_2\text{SO}_4$$

EXTENSION OF CALCULATIONS TO ATOMS OR IONS

Many of the calculations later in the course will involve mass to mole or mole to mass steps. In a few cases, it will be required to find the number of atoms or ions of one of the elements in the compound (depending upon whether it is a covalent compound or an ionic compound). The steps are the same, it is the terminology that differs. For covalent compounds, recall that the smallest unit is a molecule and that the molecule consists of combinations of atoms. The flow chart for this procedure is shown in Figure 8.2. In Chapter 4, Section 4.5, the units used for the Avogadro constant was 'atom·mol^{-1}'. When performing calculations involving covalent compounds, then the Avogadro constant has to be expressed in units of 'molecules·mol^{-1}'.

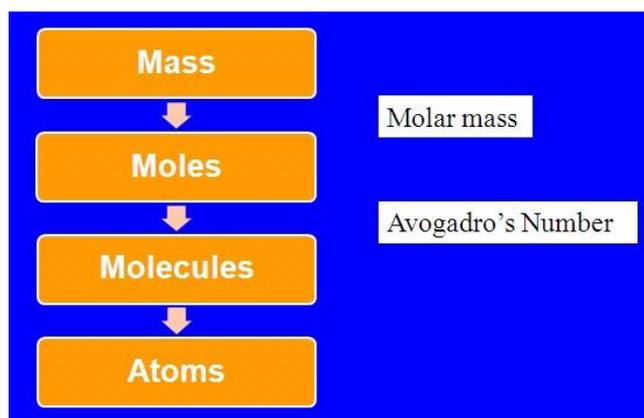Figure 8.2 The interconversion of mass, moles, molecules, and numbers of atoms for a covalent compound.

EXAMPLE 8.6

How many atoms of chlorine are there in 5.64 g of carbon tetrachloride, CCl_4?
Avogadro's constant = 6.02×10^{23} molecules·mol^{-1}

Answer

First, calculate the molar mass of CCl_4 = (1 × 12.0 g) + (4 × 35.5 g) = 154.0 g·mol^{-1}

Strategy	Relationship
Mass of CCl_4 → mol CCl_4	1 mol ≡ 154.0 g CCl_4
Mol of CCl_4 → # of molecules CCl_4	1 mol ≡ 6.02×10^{23} molecules
# of molecules CCl_4 → # of atoms Cl	1 molecule CCl_4 ≡ 4 atom Cl

$$\text{Mol of } CCl_4 = 5.64 \text{ g } CCl_4 \times \left(\frac{1 \text{ mol}}{154.0 \text{ g}}\right) = 3.66 \times 10^{-2} \text{ mol } CCl_4$$

$$\text{\# of molecules } CCl_4 = 3.66 \times 10^{-2} \text{ mol } CCl_4 \times \left(\frac{6.02 \times 10^{23} \text{ molecules}}{1 \text{ mol}}\right)$$

$$= 2.20 \times 10^{22} \text{ molecules } CCl_4$$

$$\text{\# of atom Cl} = 2.20 \times 10^{22} \text{ molecule CCl}_4 \times \left(\frac{4 \text{ atoms Cl}}{1 \text{ molecule CCl}_4} \right)$$

$$= 8.80 \times 10^{22} \text{ atoms Cl}$$

However, if it is an ionic compound, then the smallest unit is the formula unit and the formula unit consists of combinations of ions. Thus from moles it is necessary to find the number of formula units, then the number of ions (Figure 8.3). For these calculations, the Avogadro constant has to be in 'formula units·mol^{-1}' as is shown in the next calculation.
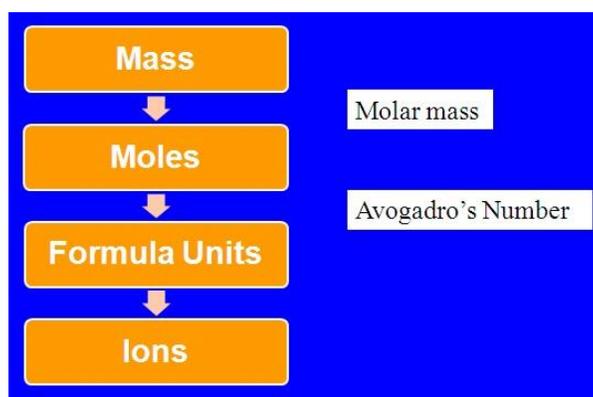

Figure 8.3 The interconversion of mass, moles, formula units, and ions for an ionic compound.

EXAMPLE 8.7

How many chloride ions are there in 8.29 g of tin(IV) chloride, $SnCl_4$?

Avogadro's constant = 6.02×10^{23} formula units·mol^{-1}

Answer

First, calculate the molar mass of $SnCl_4 = (1 \times 118.7 \text{ g}) + (4 \times 35.5 \text{ g}) = 260.7 \text{ g·mol}^{-1}$

Strategy	Relationship
Mass of $SnCl_4 \rightarrow$ mol $SnCl_4$	1 mol ≡ 260.7 g $SnCl_4$
Mol of $SnCl_4 \rightarrow$ # of formula units $SnCl_4$	1 mol ≡ 6.02×10^{23} formula units
# of formula units $SnCl_4 \rightarrow$ # of ions Cl^-	1 formula unit $SnCl_4$ ≡ 4 ions Cl^-

$$\text{Mol of SnCl}_4 = 8.29 \text{ g SnCl}_4 \times \left(\frac{1 \text{ mol}}{260.7 \text{ g}} \right) = 3.18 \times 10^{-2} \text{ mol SnCl}_4$$

$$\text{\# of formula units SnCl}_4 = 3.18 \times 10^{-2} \text{ mol SnCl}_4 \times \left(\frac{6.02 \times 10^{23} \text{ formula units}}{1 \text{ mol}} \right)$$

$$= 1.91 \times 10^{22} \text{ formula units SnCl}_4$$

$$\text{\# of ion Cl}^- = 1.91 \times 10^{22} \text{ formula units SnCl}_4 \times \left(\frac{4 \text{ ions Cl}^-}{1 \text{ formula unit SnCl}_4} \right)$$

$$= 7.66 \times 10^{22} \text{ ions Cl}^-$$

8.4 The Composition of a Compound

Each chemical compound has a specific composition. For example, common salt anywhere in the universe will contain sodium ions and chloride ions in a 1:1 ratio. This concept is known as the **Law of Constant Composition**. The Law can also be expressed as: a specific compound always contains the same elements in the same fixed ratio by mass.

It is often important to know what percentage of a particular element there is in a specific compound. Such calculations are important in the field of nutrition. The formula used for the calculation is shown below.

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

EXAMPLE 8.8

Calculate the percentage of sodium in sodium carbonate, Na_2CO_3.

Answer

First, calculate the molar mass of $Na_2CO_3 = (2 \times 23.0 \text{ g}) + (1 \times 12.0 \text{ g}) + (3 \times 16.0 \text{ g})$
$$= 106.0 \text{ g·mol}^{-1}$$

$$\text{Percent sodium} = \frac{46.0 \text{ g}}{106.0 \text{ g}} \times 100\% = 43.4\% \text{ Na}$$

8.5 Empirical and Molecular Formulas

Though it is sometimes necessary to calculate the percentage composition of a compound, an equally important task is to convert percentage composition information to the chemical formula. It is by means of this calculation that it becomes possible to determine the formula of an unknown compound.

EMPIRICAL FORMULAS

Up to now, the true, or **molecular formula**, has been used for a chemical compound. When solving this next type of calculation, it is the simplest whole-number-ratio of elements in the

compound that is determined. This is known as the ***empirical formula***. For example, hydrogen peroxide (systematic name, dihydrogen dioxide) has a molecular formula of H_2O_2, but its empirical formula is HO.

As with most chemical calculations, there is a standard method of solving empirical formula problems. Often (but not always), the information is given as percentage composition. If it is, then the first step is to assume 100.0 g of compound, in which case the percentages will be equivalent to the same mass in grams. From there, moles of each element can be calculated. The last step is to divide by the smaller/smallest number and obtain whole-number-ratios of each element. From this, the empirical formula is obtained. The next example shows the procedure in detail.

EXAMPLE 8.9

A compound of phosphorus and fluorine contains 35.2% phosphorus and 64.8% fluorine. What is the empirical formula of the compound?

Answer

Assume 100.0 g of compound. This will contain 35.2 g of phosphorus and 64.8 g of fluorine.

$$\text{Mol of P} = 35.2 \text{ g P} \times \left(\frac{1 \text{ mol}}{31.0 \text{ g}}\right) = 1.14 \text{ mol P}$$

$$\text{Mol of F} = 64.8 \text{ g F} \times \left(\frac{1 \text{ mol}}{19.0 \text{ g}}\right) = 3.41 \text{ mol F}$$

$$\text{Ratio} = \frac{1.14 \text{ mol P}}{1.14 \text{ mol}} : \frac{3.41 \text{ mol F}}{1.14 \text{ mol}} = 1 \text{ P} : 2.99 \text{ F}$$

Rounding to the nearest whole number of 1:3, gives the empirical formula of PF_3.

In the large majority of examples, the ratios are very close to integers. There are a few exceptions. This results from formulas in which there is more than one atom or ion of each element. For example, nitrogen forms an oxide of formula N_2O_3 (dinitrogen trioxide). The ratio of the two elements is 1 N:1.5 O. In such a case, the atom numbers have to be doubled to obtain the integer values of 2 N:3 O.

EXAMPLE 8.10

A compound of nitrogen and oxygen contains 25.9% nitrogen. What is the empirical formula and corresponding name of the compound?

Answer
First, by subtraction, the percentage of oxygen is 74.1%
Assume 100.0 g of compound. This will contain 25.9 g of nitrogen and 74.1 g of oxygen.

$$\text{Mol of N} = 25.9 \text{ g N} \times \left(\frac{1 \text{ mol}}{14.0 \text{ g}}\right) = 1.85 \text{ mol N}$$

$$\text{Mol of O} = 74.1 \text{ g O} \times \left(\frac{1 \text{ mol}}{16.0 \text{ g}}\right) = 4.63 \text{ mol O}$$

$$\text{Ratio} = \frac{1.85 \text{ mol N}}{1.85 \text{ mol}} : \frac{4.63 \text{ mol O}}{1.85 \text{ mol}} = 1 \text{ N} : 2.50 \text{ O}$$

Multiplying by two gives a ratio of 2 N:5 O

The empirical formula is N_2O_5 and the name is dinitrogen pentaoxide.

MOLECULAR FORMULAS

Though empirical formulas are useful, the molecular formula is much more crucial. To find this, we need the empirical formula together with the known molar mass of the compound (how to find the molar mass will be covered later in the course). The procedure is shown in Figure 8.4 below.
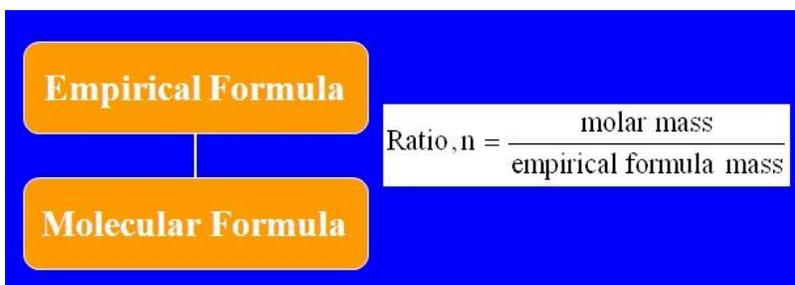

Figure 8.4 To find the molecular formula from the empirical formula, the evaluation of a mass ratio is needed.

EXAMPLE 8.11

Sulfur combines with fluorine to form a compound containing 62.8% sulfur and 37.2% fluorine. The molar mass of the compound is 102 g·mol⁻¹. Calculate the molecular formula of the compound.

Answer

Assume 100.0 g of compound. This will contain 62.8 g of sulfur and 37.2 g of fluorine.

$$\text{Mol of S} = 62.8 \text{ g S} \times \left(\frac{1 \text{ mol}}{32.1 \text{ g}}\right) = 1.96 \text{ mol S}$$

$$\text{Mol of F} = 37.2 \text{ g F} \times \left(\frac{1 \text{ mol}}{19.0 \text{ g}}\right) = 1.96 \text{ mol F}$$

$$\text{Ratio} = \frac{1.96 \text{ mol S}}{1.96 \text{ mol}} : \frac{1.96 \text{ mol F}}{1.96 \text{ mol}} = 1 \text{ S} : 1 \text{ F}$$

The empirical formula is SF. The molecular formula will be some multiple of this: $(SF)_n$. To find n, the ratio of the molar mass (102 g) and the empirical formula mass (1×32.1 g $+ 1 \times 19.0$ g $= 51.1$ g) is found. The value n is always an integer.

$$\text{Mass ratio,} \, n = \frac{102 \text{ g}}{51.1 \text{ g}} = 2$$

The molecular formula is $(SF)_2$ or more correctly, S_2F_2

8.6 Determining an Empirical Formula by Experiment

It is relatively simple to determine the empirical formula of certain compounds. These are compounds that are decomposed by heating or can be formed by reacting the elements together. The laboratory calculations are slightly different in that the masses are directly measured. Also, as the laboratory balances are precise, care must be taken in having enough significant figures for the molar mass values.

In such measurements, a weighed sample is placed in a heat-resistant container called a crucible. The crucible is strongly heated until the required chemical change has occurred. The final mass is determined and the empirical formula calculation performed. Figure 8.5 shows the typical equipment.
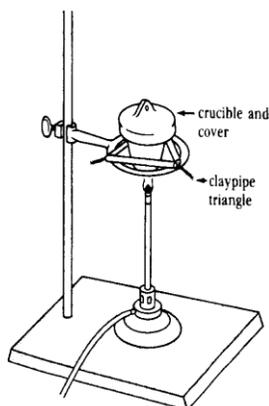
Figure 8.5 Equipment that can be used to determine the empirical formula of a compound

EMPIRICAL FORMULA OF A BINARY COMPOUND

Most commonly, the empirical formula of a metal oxide can be found by weighing out a sample of the metal, then heating it strongly to form the oxide. The mass of the metal oxide can then be obtained. The difference in the two masses will give the mass of the oxygen incorporated to form the compound. The following example is typical.

EXAMPLE 8.12

A mass of 4.5082 g of tin metal was placed in a crucible and heated strongly. After cooling the mass of the contents of the crucible was 5.7237 g. Determine the empirical formula of the compound and provide its name.

Answer

First, the mass of oxygen can be found by subtraction = (5.7237 g − 4.5082 g) = 1.2155 g
Then the empirical formula type solution is employed.

$$\text{Mol of Sn} = 4.5082 \text{ g Sn} \times \frac{(1 \text{ mol})}{(118.71 \text{ g})} = 3.7977 \times 10^{-2} \text{ mol Sn}$$

$$\text{Mol of O} = 1.2155 \text{ g O} \times \frac{(1 \text{ mol})}{(15.999 \text{ g})} = 7.5973 \times 10^{-2} \text{ mol O}$$

$$\text{Ratio} = \frac{3.7977 \times 10^{-2} \text{ mol Sn}}{3.7977 \times 10^{-2} \text{ mol}} : \frac{7.5973 \times 10^{-2} \text{ mol O}}{3.7977 \times 10^{-2} \text{ mol}} = 1 \text{ Sn} : 2.0005 \text{ O}$$

Empirical formula is SnO_2 and the corresponding name is tin(IV) oxide

DETERMINING THE FORMULA OF A HYDRATE

As introduced in Chapter 7, Section 7.9, some ionic compounds have molecules of water embedded in the crystal lattice of the compound. The number of molecules of water per one formula unit of compound can be found experimentally in a similar way to the formula of a binary compound. In this case, a known mass of the hydrate is heated gently until all of the water molecules are released from the crystal lattice as steam. After cooling, the mass of the anhydrous (water-less) compound is measured. The difference in the masses will give the mass of water. From the mass of the anhydrous compound, and the mass of water, the empirical formula can be calculated.

EXAMPLE 8.13

When 5.481 g of a hydrate of calcium chloride, $CaCl_2$, is heated gently, then cooled, 4.140 g of the anhydrous compound remain. What is the empirical formula of the compound?

Answer

First, the mass of water is needed = (5.481 g – 4.140 g) = 1.341 g

Then the empirical formula type solution is employed.

$$\text{Mol of } CaCl_2 = 4.140 \text{ g } CaCl_2 \times \frac{(1 \text{ mol})}{(111.1 \text{ g})} = 3.726 \times 10^{-2} \text{ mol } CaCl_2$$

$$\text{Mol of } H_2O = 1.341 \text{ g } H_2O \times \frac{(1 \text{ mol})}{(18.0 \text{ g})} = 7.450 \times 10^{-2} \text{ mol } H_2O$$

$$\text{Ratio} = \frac{3.726 \times 10^{-2} \text{ mol } CaCl_2}{3.726 \times 10^{-2} \text{ mol}} : \frac{7.450 \times 10^{-2} \text{ mol } H_2O}{3.726 \times 10^{-2} \text{ mol}} = 1 \, CaCl_2 : 1.999 \, H_2O$$

Empirical formula is $CaCl_2 \cdot 2H_2O$

8.7 Where Next?

In Section 8.6, Example 8.12, the empirical formula of an oxide of tin was determined by transforming shiny tin metal into its powdery white oxide, tin(IV) oxide. This process is called a chemical reaction. In the next Chapter, some of the fundamental principles of chemical reactions will be introduced.