4.5: Empirical and Molecular Formulas

In Chapter 2, we introduced the concept of a chemical compound as a substance that results from the combination of two or more atoms, in such a way that the atoms are bonded together in a constant ratio. We represented that ratio using the symbols for the atoms in the molecule, with subscripts to indicate the fixed ratios of the various atoms. The result is a molecular formula, and in Chapter 3, we used molecular formulas to devise chemical names for both molecular and ionic compounds. As we have seen in this chapter, molecular formulas can be used to directly calculate the molar mass of a compound.

Many of the methods, however, that chemists use in the laboratory to determine the composition of compounds do not give the molecular formula of the compound directly, but instead simply yield the *lowest whole-number ratio* of the elements in the compound. A formula such as this is called an **empirical formula**. For example, the molecular formula for glucose is $C_6H_{12}O_6$, but the simplest whole-number ratio of the elements in glucose is CH_2O; if you multiply each element in (CH_2O) by *six*, you obtain the molecular formula for glucose. An empirical formula cannot be converted into a molecular formula unless you know the molar mass of the compound. For example, the empirical formula for acetic acid (the acidic component in vinegar) is identical to that for glucose (CH_2O). If you analyzed these two compounds and determined only an empirical formula, you could not identify which compound you had.

Conversion of an empirical formula into a molecular formula requires that you know the molar mass of the compound in question. Knowing this, you can calculate a molecular formula based on the fact that an empirical formula can always be multiplied by an integer *n* to yield a molecular formula. Thus, some value of *n*, multiplying each element in CH_2O will yield the molecular formula of acetic acid. The value of *n* can be determined as follows:

$$n \times (CH_2O),\ where\ n = \frac{molar\ mass\ of\ the\ compound}{molar\ mass\ of\ the\ empirical\ formula}$$

For acetic acid, the molar mass is 60.05 g/mol, and the molar mass of the empirical formula CH_2O is 30.02 g/mol. The value of the integer *n* for acetic acid is therefore,

$$n = \frac{60.05\ g/mol}{30.02\ g/mol} = 2$$

And the molecular formula is $\mathbf{C_2H_4O_2}$.

Note that *n* must be an integer and that your calculation should always yield a whole number (or very close to one).

? Exercise 4.5.1

a. A compound is determined to have a molar mass of 58.12 g/mol and an empirical formula of C_2H_5; determine the molecular formula for this compound.
b. Benzene is an intermediate in the production of many important chemicals used in the manufacture of plastics, drugs, dyes, detergents and insecticides. Benzene has an empirical formula of CH. It has a molar mass of 78.11 g/mol.What is the molecular formula?