

6.8: Calculating Empirical Formulas for Compounds

Learning Objectives

- Define empirical formula.
- Determine empirical formula from percent composition of a compound.

In the early days of chemistry, there were few tools for the detailed study of compounds. Much of the information regarding the composition of compounds came from the elemental analysis of inorganic materials. The "new" field of organic chemistry (the study of carbon compounds) faced the challenge of not being able to characterize a compound completely. The relative amounts of elements could be determined, but so many of these materials had carbon, hydrogen, oxygen, and possibly nitrogen in simple ratios. We did not know exactly how many of these atoms were actually in a specific molecule.

Determining Empirical Formulas

An empirical formula tells us the relative ratios of different atoms in a compound. The ratios hold true on the *molar* level as well. Thus, H_2O is composed of two atoms of hydrogen and 1 atom of oxygen. Likewise, **1.0 mole of H_2O is composed of 2.0 moles of hydrogen and 1.0 mole of oxygen.** We can also work backwards from molar ratios because *if we know the molar amounts of each element in a compound, we can determine the empirical formula.*

*In a procedure called **elemental analysis**, an unknown compound can be analyzed in the laboratory in order to determine the percentages of each element contained within it. These percentages can be transformed into the mole ratio of the elements, which leads to the empirical formula.*

Empirical Formula: In Steps

Steps to determine empirical formula:

1. Assume a 100 g sample of the compound so that the given percentages can be directly converted into grams.
2. Use each element's molar mass to convert the grams of each element to moles.
3. In order to find a whole-number ratio, divide the moles of each element by whichever of the moles from step 2 is the smallest.
4. If all the moles at this point are whole numbers (or very close), the empirical formula can be written with the moles as the subscript of each element.
5. In some cases, one or more of the moles calculated in step 3 will not be whole numbers. Multiply each of the moles by the smallest whole number that will convert each into a whole number. Write the empirical formula.

Example 6.8.1

A compound of iron and oxygen is analyzed and found to contain 69.94% iron and 30.06% oxygen. Find the empirical formula of the compound.

Solution

Solutions to Example 6.8.1

Steps for Problem Solving	Find the empirical formula of a compound of 69.94% iron and 30.06% oxygen.
Identify the "given" information and what the problem is asking you to "find."	Given: % of Fe = 69.94% % of O = 30.06% Find: Empirical formula = Fe_xO_y
Calculate	

Steps for Problem Solving

Find the empirical formula of a compound of 69.94% iron and 30.06% oxygen.

a. Assume a 100 g sample, convert the same % values to grams.

69.94 g Fe

30.06 g O

b. Convert to moles.

$$69.94 \text{ g Fe} \times \frac{1 \text{ mol Fe}}{55.85 \text{ g Fe}} = 1.252 \text{ mol Fe}$$

$$30.06 \text{ g O} \times \frac{1 \text{ mol O}}{16.00 \text{ g O}} = 1.879 \text{ mol O}$$

c. Divide both moles by the smallest of the results.

$$\text{Fe} : \frac{1.252 \text{ mol}}{1.252}$$

$$\text{O} : \frac{1.879 \text{ mol}}{1.252}$$

The "non-whole number" empirical formula of the compound is $\text{Fe}_1\text{O}_{1.5}$

Multiply each of the moles by the smallest whole number that will convert each into a whole number.

$$\text{Fe}:\text{O} = 2 (1:1.5) = 2:3$$

Since the moles of O is still not a whole number, both moles can be multiplied by 2, while rounding to a whole number.

Write the empirical formula.

The empirical formula of the compound is Fe_2O_3 .

Think about your result.

The subscripts are whole numbers and represent the mole ratio of the elements in the compound. The compound is the ionic compound iron (III) oxide.

? Exercise 6.8.1

Mercury forms a compound with chlorine that is 73.9% mercury and 26.1% chlorine by mass. What is the empirical formula?

Answer



Summary

- A process is described for the calculation of the empirical formula of a compound, based on the percent composition of that compound.

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