Empirical and Molecular Formulas

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CONCEPT 1 Empirical and Molecular Formulas

Lesson Objectives

The student will:

- reduce molecular formulas to empirical formulas.
- determine the empirical formula of a compound given either percent composition or masses.
- determine the molecular formula of a compound given either percent composition and molar mass or masses.

Vocabulary

- molecular formula

Introduction

The empirical formula is the simplest ratio of atoms in a compound. Formulas for ionic compounds are always empirical formulas, but for covalent compounds, the empirical formula is not always the actual formula for the molecule. Molecules such as benzene, C_6H_6, would have an empirical formula of CH.

Finding Empirical Formula from Experimental Data

Empirical formulas can be determined from experimental data or from percent composition. Consider the following example.

Example:

We find that a 2.50 gram sample of a compound contains 0.900 grams of calcium and 1.60 grams of chlorine. The compound contains only these two elements. We can calculate the number of moles of calcium and chlorine atoms in the compound. We can then find the molar ratio of calcium atoms to chlorine atoms. From this, we can determine the empirical formula.

Solution:

First, we convert the mass of each element into moles.

$$\text{moles of Ca} = \frac{0.900\text{ g}}{40.1\text{ g/mol}} = 0.0224\text{ mol Ca}$$
$$\text{moles of Cl atoms} = \frac{1.60\text{ g}}{35.5\text{ g/mol}} = 0.0451\text{ mol Cl}$$

At this point, we have the correct ratio for the atoms in the compound. The formula $Ca_{0.0224}Cl_{0.0451}$, however, isn't acceptable. We need to find the simplest *whole* number ratio. To find a simple whole number ratio for these numbers, we divide each of them by the smaller number.

$$\text{Ca} = \frac{0.0224}{0.0224} = 1.00 \qquad \text{Cl} = \frac{0.0451}{0.0224} = 2.01$$

Now, we can see the correct empirical formula for this compound is $CaCl_2$.

Finding Empirical Formula from Percent Composition

When finding the empirical formula from percent composition, the first thing to do is to convert the percentages into masses. For example, suppose we are given that the percent composition of a compound as 40.0% carbon, 6.71% hydrogen, and 53.3% oxygen. Since every sample of this compound will have the same composition in terms of the ratio of atoms, we could choose a sample of any size. Suppose we choose a sample size of 100. grams. The masses of each of the elements in this sample will be 40.0 grams of carbon, 6.71 grams of hydrogen, and 53.3 grams of oxygen. These masses can then be used to find the empirical formula. You could use any size sample, but choosing a sample size of 100. grams is usually most convenient because it makes the arithmetic simple.

Example:

Find the empirical formula of a compound whose percent composition is 40.0% carbon, 6.71% hydrogen, and 53.3% oxygen.

Solution:

We choose a sample size of 100. grams and multiply this 100. gram sample by each of the percentages to get masses for each element. This would yield 40.0 grams of carbon, 6.71 grams of hydrogen, and 53.3 grams of oxygen. The next step is to convert the mass of each element into moles.

$$\begin{aligned}
\text{moles of C} &= \frac{40.0 \text{ g}}{12.0 \text{ g/mol}} = 3.33 \text{ moles C} \\
\text{moles of H} &= \frac{6.71 \text{ g}}{1.01 \text{ g/mol}} = 6.64 \text{ moles H} \\
\text{moles of O} &= \frac{53.3 \text{ g}}{16.0 \text{ g/mol}} = 3.33 \text{ mole Ca}
\end{aligned}$$

Then, we divide all three numbers by the smallest one to get simple whole number ratios:

$$\text{C} = \frac{3.33}{3.33} = 1 \qquad \text{H} = \frac{6.64}{3.33} = 2 \qquad \text{O} = \frac{3.33}{3.33} = 1$$

Finally, we can write the empirical formula CH_2O.

Sometimes, this technique of dividing each of the moles by the smallest number does not yield whole numbers. Whenever the subscript for any element in the empirical formula is 1, dividing each of the moles by the smallest will yield a simple whole number ratio, but if none of the elements in the empirical formula has a subscript of 1, then this technique will not yield a simple whole number ratio. In those cases, a little more work is required.

Example:

Determine the empirical formula for a compound that is 66.0% calcium and 34.0% phosphorus.

Solution:

We choose a sample size of 100. grams and multiply the 100. grams by the percentage of each element to get masses. This yields 66.0 grams of calcium and 34.0 grams of phosphorus. We then divide each of these masses by their molar mass to convert the masses into moles:

$$\text{moles of Ca} = \frac{66.0 \text{ g}}{40.1 \text{ g/mol}} = 1.65 \text{ moles Ca}$$
$$\text{moles of P} = \frac{34.0 \text{ g}}{31.0 \text{ g/mol}} = 1.10 \text{ moles P}$$

We then divide each of these moles by the smallest.

$$\text{Ca} = \frac{1.65}{1.10} = 1.50 \qquad \text{P} = \frac{1.10}{1.10} = 1.00$$

In this case, dividing each of the numbers by the smallest one does not yield a simple whole number ratio. In such a case, we must multiply both numbers by some factor that will produce a whole number ratio. If we multiply each of these by 2, we get a whole number ratio of 3 Ca to 2 P. Therefore, the empirical formula is Ca_3P_2.

Finding Molecular Formulas

Empirical formulas show the simplest whole number ratio of the atoms in a compound. Molecular formulas show the actual number of atoms of each element in a compound. When you find a empirical formula from either masses of elements or from percent composition, you are finding the empirical formula. For the compound N_2H_4, you will get an empirical formula of NH_2, and for C_3H_6, you will get CH_2. If we want to determine the actual molecular formula, we need one additional piece of information. The molecular formula is always a whole number multiple of the empirical formula. In order to get the molecular formula for N_2H_4, you must double each of the subscripts in the empirical formula. Since the molecular formula is a whole number multiple of the empirical formula, the molecular mass will be the same whole number multiple of the formula mass. The formula mass for NH_2 is 16 g/mol, and the molecular mass for N_2H_4 is 32 g/mol. When we have the empirical formula and the molecular mass for a compound, we can divide the formula mass into the molecular mass and find the whole number that we need to multiply each of the subscripts in the empirical formula.

Example:

Find the molecular formula for a compound with percent composition of 40.0% carbon, 67.1% hydrogen, and 53.3% oxygen. The molecular mass of the compound is 180 g/mol.

Solution:

This is the same as an earlier example, except now we also have the molecular mass of the compound. Earlier, we determined the empirical formula of this compound to be CH_2O. The empirical formula has a formula mass of 30.0 g/mol. In order to find the molecular formula for this compound, we divide the formula mass into the molecular mass (180 divided by 30) and find the multiplier for the empirical formula to be 6. As a result, the molecular formula for this compound will be $C_6H_{12}O_6$.

Example:

Find the molecular formula for a compound with percent composition of 85.6% carbon and 14.5% hydrogen. The molecular mass of the compound is 42.1 g/mol.

Solution:

We choose a sample size of 100. g and multiply each element percentage to get masses for the elements in this sample. This yields 85.6 g of C and 14.5 g of H. Dividing each of these by their atomic mass yields 7.13 moles of C and 14.4 moles of H. Dividing each of these by the smallest yields a whole number ratio of 1 carbon to 2 hydrogen. Thus, the empirical formula will be CH_2.

The formula mass of CH_2 is 14 g/mol. Dividing 14 g/mol into the molecular mass of 42.1 g/mol yields a multiplier of 3. The molecular formula will be C_3H_6.

Lesson Summary

- The empirical formula of a compound indicates the simplest whole number ratio of atoms present in the compound.
- The empirical formula of a compound can be calculate from the masses of the elements in the compound or from the percent composition.
- The molecular formula of a compound is some whole number multiple of the empirical formula.

Further Reading / Supplemental Links

This website has solved example problems for a number of topics covered in this lesson, including the determination of empirical and molecular formulas.

- http://www.sciencejoywagon.com/chemzone/05chemical-reactions/

Review Questions

1. What is the empirical formula for C_8H_{18}?
2. What is the empirical formula for C_6H_6?
3. What is the empirical formula for WO_2?
4. A compound has the empirical formula C_2H_8N and a molar mass of 46 g/mol. What is the molecular formula of this compound?
5. A compound has the empirical formula C_2H_4NO. If its molar mass is 116.1 g/mol, what is the molecular formula of the compound?
6. A sample of pure indium chloride with a mass of 0.5000 grams is found to contain 0.2404 grams of chlorine. What is the empirical formula of this compound?
7. Determine the empirical formula of a compound that contains 63.0 grams of rubidium and 5.90 grams of oxygen.
8. Determine the empirical formula of a compound that contains 58.0%Rb, 9.50%N, and 32.5%O.
9. Determine the empirical formula of a compound that contains 33.3%Ca, 40.0%O, and 26.7%S.
10. Find the molecular formula of a compound with percent composition 26.7%P, 12.1%N, and 61.2%Cl and with a molecular mass of 695 g/mol.