

EMPIRICAL AND MOLECULAR FORMULAS

A compound never before seen has just been prepared in a chemistry lab. What is the formula for that compound? In order to answer that question, a chemist must first determine the percent composition of the compound. From this information, the chemist can then determine the compound's empirical formula. The empirical formula of a compound shows the simplest whole-number ratio of elements present in the compound. The first step in determining an empirical formula is to calculate the number of moles of each element present in the compound. Next, you must find the mole ratio of the elements in the compound by dividing the number of moles of each element by the smallest number of moles. The whole-number ratio you obtain gives you the subscripts for the empirical formula of the compound. The molecular formula may be the same as the empirical formula or some whole-number multiple of the empirical formula. In order to determine a compound's molecular formula, you need to know both the empirical formula and the formula mass of that compound.

Example: Analysis of a compound shows that it contains 10.88 g of calcium and 19.07 g of chlorine. Determine the empirical formula of this compound.

Solution: Start by converting the mass of each element to its equivalent in moles:

$$19.07 \text{ g Cl} \times \frac{1 \text{ mol Cl}}{35.45 \text{ g Cl}} = 0.5408 \text{ mol Cl}$$

$$10.88 \text{ g Ca} \times \frac{1 \text{ mol Ca}}{40.08 \text{ g Ca}} = 0.2715 \text{ mol Ca}$$

Now calculate the mole ratio between the two elements by dividing both of the above numbers by the smaller of the two (0.2715 mol Ca is the smaller number, so that is the divisor).

$$\frac{0.5408 \text{ mol Cl}}{0.2715} = 1.9919 \text{ mol Cl} \qquad \frac{0.2715 \text{ mol Ca}}{0.2715} = 1.000 \text{ mol Ca}$$

The mole ratio of the two elements, then, is nearly 2:1. *If it is within 0.1 you may round off the number to the nearest whole number.* Therefore, the empirical formula for the compound is CaCl_2 .

- Determine the empirical formula of a certain copper sulfide ore if a 7.68 g sample of the compound contains 6.13 g of copper.
- Calculate the molecular formula of a compound containing 24.1 g of carbon and 5.1 g of hydrogen. The molar mass of this compound is known to be 58.1 g/mol.
 Solution Directions:
 - Convert the mass of each element to moles
 - Find the empirical formula (remembering to round off to nearest whole number if within 0.1)
 - Calculate the mass of the empirical formula.
 - If this mass is equal to the molar mass then the empirical formula = molecular formula
 - If this mass differs, divide it into the molecular mass to determine the appropriate multiple of the empirical formula.
 - Multiply this number times each of the subscripts of the empirical formula to determine the molecular formula.
- Determine the empirical formula of a compound that contains 69.5 % oxygen and 30.5% nitrogen. *Remember that you may consider this 69.5 grams of oxygen and 30.5 g of nitrogen in a 100 gram sample. Convert these grams of elements to moles and continue the process to determine the empirical formula.*
- Determine the empirical formula of a compound with a percent composition of 29.1% Na, 40.5% S and 30.4% O.
- Calculate the empirical formula for each compound:
 - 7.8% carbon and 92.2% chlorine
 - 10% C, 0.8% H, 89.1% Cl
 - 30.4% N and 69.6% O
 - 22.6% N and 77.4% O
- The formula mass of a compound is 166.3 g. The compound contains 47.1% potassium, 14.5% carbon and 38.4% oxygen. What is the molecular formula for the compound?

PERCENT COMPOSITION

Chemists often have to determine the percent composition of a compound. Percent composition refers to the number of grams of each element in a compound present in 100 g of that compound. Knowing a compound's percent composition is the first step in determining the formula of that compound. Percent composition is determined in the laboratory by analyzing a sample of the compound to see what mass of each element is present in the compound. Then for each element:

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

Example A

A compound analyzed in a chemistry laboratory consists of 5.34 g of carbon, 0.42 g of hydrogen, and 47.08 g of chlorine. What is the percent composition of this compound?

Solution: The total mass of the compound is equal to the sum of the masses of the three elements that make it up:

$$\begin{aligned} \text{Mass of compound} &= \text{mass of C} + \text{mass of H} + \text{mass of Cl} \\ &= 5.34 \text{ g} + 0.42 \text{ g} + 47.08 \text{ g} \\ &= 52.84 \text{ g} \end{aligned}$$

Then the percent of each element in the compound is calculated as follows:

$$\begin{aligned} \text{Percent C} &= \frac{\text{mass of the element}}{\text{total mass of the compound}} \times 100\% \\ &= \frac{5.34 \text{ g C}}{52.84 \text{ g cmpd}} \times 100\% = 10.1\% \text{ C} \\ \text{Percent H} &= \frac{0.42 \text{ g H}}{52.84 \text{ g cmpd}} \times 100\% = 0.79\% \text{ H} \\ \text{Percent Cl} &= \frac{47.08 \text{ g Cl}}{52.84 \text{ g cmpd}} \times 100\% = 89.1\% \end{aligned}$$

- Find the percent composition of a compound containing tin and chlorine if 18.35 g of the compound contains 5.74 g of tin.
- Determine the percent composition of ammonia from its formula, NH_3 .
- Calculate the percent of each element present in potassium phosphate from its formula, K_3PO_4 .
- Determine the percent composition of a compound that consists of 3.907 g of carbon and 0.874 g of hydrogen.
- From the formula for calcium acetate, $\text{Ca}(\text{C}_2\text{H}_3\text{O}_2)_2$, calculate the mass of carbon that can be obtained from 65.3 g of the compound.