Simple vs. True
Calculating Empirical and Molecular Formulas

Formula writing is a key component for success in chemistry. How do scientists really know what the "true" formula for a compound might be? In this lesson we will explore some of the mathematics supporting many of the chemical formulas that you have encountered.

PURPOSE
In this lesson you will learn problem-solving strategies that will enable you to calculate empirical and molecular formulas given experimental data.

MATERIALS
calculator
periodic table

CLASS NOTES
The simplest formula, *empirical formula*, for a compound is the smallest whole number ratio of atoms present in a given formula. The *molecular formula* represents the true ratio of atoms in a molecular compound. Sometimes the empirical formula and the molecular formula are the same. For example, the formula for water, H_2O, is both the simplest ratio of elements and the true ratio of elements. In other instances, the molecular formula is a whole number multiple of the empirical formula. For example, the formula for butane is C_4H_{10}. This formula represents the molecular formula, the true ratio of atoms. The empirical formula for this compound is easily found by reducing the subscripts (dividing by the greatest common factor) to end with C_2H_5. For ionically-bonded substances, the empirical formula is the representation that is commonly written as the formula. For example, in the formula NaCl, Na and Cl are in a 1:1 ratio in this empirical formula, however, sodium chloride crystals are actually face-centered cubic in shape and one unit cell requires many more than 2 ions while maintaining the 1:1 ratio.

When a new substance is found or discovered, the formula is unknown until some qualitative and quantitative analyses are performed on the compound. First, qualitative analysis might reveal which elements are in the compound and then quantitatively, the amounts of those elements in the compound must be found. From this type of experimental data, the empirical formula may be calculated. Use the following strategies to make calculating empirical and molecular formulas a breeze!

EMPIRICAL FORMULA

1. Convert the percentage or grams of each element into moles. (Remember that the sum of the percentages must total 100% so by assuming a 100. gram sample, you can simply drop the % and replace it with grams. For example, if a compound has 20.0% Na, then convert this to 20.0 grams of sodium.) Leave answers to at least 4 significant figures in this step. Rounding early could yield incorrect answers later.

2. Set up a mole ratio for each element. Divide each of the moles calculated by the element with the smallest number of moles. This step may yield whole numbers. If so, these whole numbers are the subscripts for the formula.
   a. If the numbers are not whole numbers you may have to multiply by some factor (try multiplying by 2 first, then by 3, etc.) to make them whole numbers. Don't just round!

   b. For example: If the ratio comes out 1: 2.5: 1—multiplying each number by 2 will yield the same proportion with no decimals. The ratio becomes 2: 5: 2. Remember that subscripts must be whole numbers.

   c. Watch for numbers that have the following terminal decimals:
      - 0.20 (could be multiplied by 5 to yield whole numbers)
      - 0.25 (could be multiplied by 4 to yield whole numbers)
      - 0.33 (could be multiplied by 3 to yield whole numbers)
      - 0.50 (could be multiplied by 2 to yield whole numbers)

3. Write the formula with proper subscripts and name the compound if asked. (Usually the elements will be listed in order within the problem.)

EXAMPLE PROBLEM 1:

Many of the chemicals in our body consist of the elements carbon, hydrogen, oxygen and nitrogen. One of these chemicals, norepinephrine, is often released during stressful times and serves to increase our metabolic rate. The percent composition of this hormone is 56.8% C, 6.56% H, 28.4% O, and 8.28% N. Calculate the simplest formula for this biological compound.

EXAMPLE PROBLEM 2:
A sample of a white, granular ionic compound weighing 41.764 grams was found in the photography lab. Analysis of this compound revealed that the compound was composed of 12.144 grams of sodium, 16.948 grams of sulfur, and the rest of the compound was oxygen. Calculate the formula for this compound and name it!

MOLECULAR FORMULA
It may be necessary for you to calculate the empirical formula first in order to determine the molecular formula.

1. Divide the molecular mass by the empirical formula mass. This should yield a whole number.

2. Multiply all of the subscripts in the empirical formula by the whole number obtained from the previous step to get the true ratio of atoms in the molecular formula.

EXAMPLE PROBLEM 3:
Calculate the molecular formula for an organic compound whose molecular mass is 180. grams/mole and has an empirical formula of CH_2O. Name this compound.

EXAMPLE PROBLEM 4:
An organic alcohol was quantitatively found to be contain the following elements in the given proportions: C = 64.81% ; H = 13.60%; O = 21.59%

Given that the molecular weight of this alcohol is 74 g/mole, find the molecular formula and name this alcohol.

Name _____

Period _____

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ANALYSIS

Solve the following problems on this answer page. Be sure to show all work for full credit paying special attention to significant figures and units.

1. A 2.676 gram sample of an unknown compound was found to contain 0.730 g of sodium, 0.442 g of nitrogen and 1.504 g of oxygen. Calculate the empirical formula for this compound and name it.

2. A mysterious white powder was found on the kitchen counter. It was found quantitatively to contain 27.37% sodium, 1.20% hydrogen, 14.30% carbon, and the rest was found to be oxygen. Calculate the empirical formula for this compound and name it.

3. A common organic solvent has an empirical formula of CH and a molecular mass of 78 g/mole. Calculate the molecular formula for this compound and name it.

4. A gas was qualitatively analyzed and found to contain only the elements nitrogen and oxygen. The compound was further analyzed to discover that the gas was composed of 30.43% nitrogen. Given that the molecular mass of the compound is 92.0 g/mole, calculate the molecular formula.