Simple vs. True
Calculating Empirical and Molecular Formulas

OBJECTIVE
Students will learn to calculate empirical and molecular formulas and practice applying logical problem-solving skills.

LEVEL
Chemistry

NATIONAL STANDARDS
UCP.1, UCP.2, UCP.3, B.2

CONNECTIONS TO AP
AP Chemistry:
III. Reactions B. Stoichiometry 3. Mass and volume relations with emphasis on the mole concept, including empirical formulas

TIME FRAME
45 minutes

MATERIALS
calculator
periodic table
student white boards (optional)

TEACHER NOTES
This lesson is designed to be an integral part of the classroom unit involving the mole concept. It is best placed after students have mastered percent composition calculations. The student notes provide the basis for your lecture concerning empirical formula and molecular formulas. The examples easily serve as guided practice. If student white boards are available, it is a good idea to use them to engage and monitor the students. Be sure to explain each problem-solving step of the example problems; the solutions follow.

Once students have mastered the concept of converting the given quantities to moles in search of a mole:mole ratio, encourage the use of the graphing calculator to allow students to visualize the data and better understand the simplified, yet whole number mole:mole ratio.

EXAMPLE PROBLEM 1:
Many of the biochemicals 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 during the "fight or flight" response. 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.

Step 1: Convert the percent composition data of each element to moles of each element. (Assume a 100. gram sample)

$$56.8\,\cancel{g}\ C \times \frac{1\,mol\,C}{12.01\,\cancel{g}\,C} = 4.729\ mol\ C$$

$$6.56\cancel{g}\,H \times \frac{1\,mol\,H}{1.01\,\cancel{g}\,H} = 6.495\ mol\ H$$

$$28.4\,\cancel{g}\ O \times \frac{1\,mol\,O}{16.00\cancel{g}\,O} = 1.775\,mol\,O$$

$$8.28\cancel{g}\,N \times \frac{1\,mol\,N}{14.01\cancel{g}\,N} = 0.5910\,mol\,N$$

Step 2: Calculate the mole:mole ratio. The smallest number of moles calculated corresponds to nitrogen so, divide *all* of the moles calculated by nitrogen's number of moles, 0.5910 to obtain a simplified ratio.

$$\frac{4.729\,mol\,C}{0.5910\,mol\,N} = 8$$

$$\frac{6.495\,mol\,H}{0.5910\,mol\,N} = 11$$

Empirical Formula = $C_8H_{11}O_3N$

$$\frac{1.775\,mol\,O}{0.5910\,mol\,N} = 3$$

$$\frac{0.5910\,mol\,N}{0.5910\,mol\,N} = 1$$

EXAMPLE PROBLEM 2:

A sample of a white, granular ionic compound having a mass of 41.764 grams was found in the photography lab. Analysis of this compound revealed that it was composed of 12.144 grams of sodium, 16.948 grams of sulfur, and the rest of the compound was oxygen. Calculate the empirical formula for this compound and provide its name.

Step 1: Convert the data given for each element to moles of each element.

$$12.144\ \cancel{g}\ \text{Na} \times \frac{1\ \text{mol Na}}{22.99\ \cancel{g}\ \text{Na}} = 0.5282\ \text{mol Na}$$

$$16.948\ \cancel{g}\ \text{S} \times \frac{1\ \text{mol S}}{32.07\ \cancel{g}\ \text{S}} = 0.5285\ \text{mol S}$$

Calculate the grams of oxygen relying on the Law of Conservation of Mass. The total mass for the compound is 41.764 g.

$$41.764\ \text{g} - (12.144\ \text{g} + 16.948\ \text{g}) = 12.672\ \text{g O}$$

$$12.672\ \cancel{g}\ \text{O} \times \frac{1\ \text{mol O}}{16.00\ \cancel{g}\ \text{O}} = 0.792\ \text{mol O}$$

Step 2: Calculate the mole:mole ratio. The smallest number of moles calculated corresponds to sodium so, divide *all* of the moles calculated by sodium's number of moles, 0.5282 to obtain a simplified ratio.

$$\frac{0.5282\ \text{mol Na}}{0.5282\ \text{mol Na}} = 1$$

$$\frac{0.5286\ \text{mol S}}{0.5282\ \text{mol Na}} = 1$$

$$\frac{0.792\ \text{mol O}}{0.5282\ \text{mol Na}} = 1.499 = 1.5$$

Multiply all of the moles in the mole:mole ratio by 2 to obtain small whole numbers. The empirical formula becomes $Na_2S_2O_3$ $\therefore$ the compound is sodium thiosulfate.

EXAMPLE PROBLEM 3:

Calculate the molecular formula for an organic compound whose molecular mass is $180.\frac{g}{mol}$ and has an empirical formula of CH_2O. Name this compound.

<u>Step 1:</u> First, calculate the empirical mass for CH_2O.

$$12.01 + 2(1.01) + 16.00 = 30.03\frac{g}{mol}$$

Next, simplify the ratio of the molecular mass:empirical mass.

$$\frac{\text{molecular mass}}{\text{empirical mass}} = \frac{180.}{30.03} \cong 6$$

<u>Step 2:</u> Multiply the empirical formula by the factor determined in Step 1 and solve for the new subscripts.

$$6\left(CH_2O\right) = C_6H_{12}O_6 = \text{glucose}$$

EXAMPLE PROBLEM 4:
An organic alcohol was quantitatively found to 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/mol, determine the molecular formula and name this alcohol.

Step 1: Convert the percent composition data of each element to moles of each element. (Assume a 100. gram sample)

$$64.81\cancel{g}\ C \times \frac{1\,mol\,C}{12.01\cancel{g}\,C} = 5.396\,mol\,C$$

$$13.60\,\cancel{g}\,H \times \frac{1\,mol\,H}{1.01\cancel{g}\,H} = 13.47\,mol\,H$$

$$21.59\,\cancel{g}\,O \times \frac{1\,mol\,O}{16.00\,\cancel{g}\,O} = 1.349\,mol\,O$$

Step 2: Calculate the mole:mole ratio. The smallest number of moles calculated corresponds to oxygen so, divide *all* of the moles calculated by oxygen's number of moles, 1.349 to obtain a simplified ratio.

$$\frac{5.396\,mol\,C}{1.349\,mol\,O} = 4$$

$$\frac{13.47\,mol\,H}{1.349\,mol\,O} = 10$$

$$\frac{1.349\,mol\,O}{1.349\,mol\,O} = 1$$

The empirical formula is $C_4H_{10}O$ but, this is an alcohol thus written as C_4H_9OH .

Step 3: First, calculate the empirical mass for C_4H_9OH .

$$4(12.01)+10(1.01)+16.00 = 74.14\frac{g}{mol}$$

Next, simplify the ratio of the molecular mass:empirical mass.

$$\frac{molecular\ \ mass}{empirical\ \ mass} = \frac{74}{74.14} \cong 1$$

Since the empirical and molecular masses are the same, the alcohol is butanol.

ANSWERS TO THE ANALYSIS QUESTIONS

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.

<u>Step 1:</u> Convert the given data for each element to moles of each element.

$$0.730\ \cancel{g}\ \text{Na} \times \frac{1\,\text{mol Na}}{22.99\ \cancel{g}\ \text{Na}} = 0.03175\ \text{mol Na}$$

$$0.442\ \cancel{g}\ \text{N} \times \frac{1\,\text{mol N}}{14.01\ \cancel{g}\,\text{N}} = 0.03155\,\text{mol N}$$

$$1.504\ \cancel{g}\ \text{O} \times \frac{1\,\text{mol O}}{16.00\ \cancel{g}\ \text{O}} = 0.9400\,\text{mol O}$$

<u>Step 2:</u> Calculate the mole:mole ratio. The smallest number of moles calculated corresponds to nitrogen so, divide *all* of the moles calculated by nitrogen's number of moles, 0.03155 to obtain a simplified ratio.

$$\frac{0.03175\,\text{mol Na}}{0.03155\,\text{mol N}} = 1$$

$$\frac{0.03155\,\text{mol N}}{0.03155\,\text{mol N}} = 1$$

$$\frac{0.09400\,\text{mol O}}{0.03155\,\text{mol N}} = 3$$

Therefore, the empirical formula is $NaNO_3$, sodium nitrate.

2. A mysterious white powder was found at a crime scene. It was quantitatively analyzed and its percent composition was determined to be 27.37% sodium, 1.20% hydrogen, 14.30% carbon with the remainder being oxygen. Calculate the empirical formula for this compound and name it.

Step 1: Convert the percent composition data of each element to moles of each element. (Assume a 100. gram sample)

$$27.37\cancel{g}\text{ Na} \times \frac{1\text{ mol Na}}{22.99\ \cancel{g}\text{ Na}} = 1.191\text{ mol Na}$$

$$1.20\ \cancel{g}\text{ H} \times \frac{1\text{ mol H}}{1.01\cancel{g}\text{ H}} = 1.188\text{ mol H}$$

$$14.30\ \cancel{g}\text{ C} \times \frac{1\text{ mol C}}{12.01\cancel{g}\text{ C}} = 1.191\text{ mol C}$$

Calculate the percent of oxygen present. $\%\text{ oxygen} = 100 - (27.37 + 1.20 + 14.30) = 57.13\ \%$

$$57.13\ \cancel{g}\text{ O} \times \frac{1\text{ mol O}}{16.00\ \cancel{g}\text{ O}} = 3.571\text{ mol O}$$

Step 2: Calculate the mole:mole ratio. The smallest number of moles calculated corresponds to hydrogen so, divide *all* of the moles calculated by hydrogen's number of moles, 1.188 to obtain a simplified ratio.

$$\frac{1.191\text{ mol Na}}{1.188\text{ mol H}} = 1$$

$$\frac{1.188\text{ mol H}}{1.188\text{ mol H}} = 1$$

$$\frac{1.191\text{ mol C}}{1.188\text{ mol H}} = 1$$

$$\frac{3.571\text{ mol O}}{1.188\text{ mol H}} = 3$$

Therefore, the empirical formula is $NaHCO_3$, and the compound is known as either sodium bicarbonate or sodium hydrogen carbonate.

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.

Step 1: First, calculate the empirical mass for CH

$$12.01 + 1.01 = 13.04 \frac{\text{g}}{\text{mol}}$$

Next, simplify the ratio of the molecular mass: empirical mass.

$$\frac{\text{molecular mass}}{\text{empirical mass}} = \frac{78.}{13.3} \cong 6$$

Step 2: Multiply the empirical formula by the factor determined in Step 1 and solve for the new subscripts.

$6(CH) = C_6H_6$ which is known as benzene.

*Students may have to look up the name of this solvent.

4. A gas was qualitatively analyzed and found to contain only the elements nitrogen and oxygen. The compound was further analyzed and it was determined 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.

   Step 1: Convert the given data for each element to moles of each element. (Assume a 100. g sample).

$$30.43\cancel{g}\text{ N} \times \frac{1\text{ mol N}}{14.01\cancel{g}\text{ N}} = 2.172\text{ mol N}$$

Calculate the percentage of oxygen in the sample: $100\% - 30.43\% = 69.57\%$ oxygen

$$69.57\cancel{g}\text{ O} \times \frac{1\text{ mol O}}{16.00\cancel{g}\text{ O}} = 4.348\text{ mol O}$$

   Step 2: Calculate the mole:mole ratio. The smallest number of moles calculated corresponds to nitrogen so, divide *all* of the moles calculated by nitrogen's number of moles, 2.172 to obtain a simplified ratio.

$$\frac{2.172\text{ mol N}}{2.172\text{ mol N}} = 1$$

$$\frac{4.348\text{ mol O}}{2.172\text{ mol N}} = 2$$

The empirical formula is NO_2

   Step 3: First, calculate the empirical mass for NO_2.

$$14.01 + 2(16.00) = 46.01\frac{\text{g}}{\text{mol}}$$

Next, simplify the ratio of the molecular mass: empirical mass.

$$\frac{\text{molecular mass}}{\text{empirical mass}} = \frac{92}{46.01} \cong 2$$

Multiply the empirical formula by the factor determined in Step 3 and solve for the new subscripts. The actual compound is N_2O_4, dinitrogen tetroxide.

Simple vs. True
Calculating Empirical and Molecular Formulas

How do chemists determine the true chemical formula for a newly synthesized or unknown compound? In this lesson we will explore some of the mathematics chemists apply to experimental evidence to quickly and accurately determine the true chemical formula of a compound.

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
student white boards (optional)

CLASS NOTES
The simplest formula or *empirical formula* for a compound represents the smallest whole number ratio of atoms present in a given chemical substance. The *molecular formula* represents the true ratio of atoms actually present in a molecular compound. Sometimes the empirical formula and the molecular formula are identical. For example, the formula for water, H_2O, is both the simplest ratio of atoms contained per molecule of water as well as the true ratio. 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, which is the true ratio of atoms present in a molecule of butane. The empirical formula for this compound is easily determined by reducing the subscripts to the simplest whole number ratio possible. This is accomplished by dividing all of the subscripts by the greatest common factor, which is 2, to yield C_2H_5. For ionically-bonded substances, the empirical formula is the representation of the smallest formula unit. For example, in the formula NaCl, Na and Cl are in a 1:1 ratio, however, sodium chloride crystals are actually arranged in a crystal lattice that is face-centered cubic. One unit cell requires many more ions yet maintains the 1:1 ion to ion ratio.

When a new substance is discovered, the formula is unknown until some qualitative and quantitative analyses are performed on the compound. First, qualitative analysis reveals which elements are in the compound. Next, quantitative analysis determines the amounts of those elements in the compound. Chemists use this type of experimental data to determine the empirical formula. Additional data must be collected in order to determine the molecular formula.

CALCULATING EMPIRICAL FORMULAS

1. Convert the grams given for each element into moles. If the data is given as percent composition data, it is simplest to assume a 100g sample so that each percentage is converted directly to grams. For example, if a compound contains 20.0% Na, then convert this directly to 20.0 grams of sodium and then convert the quantity into moles of sodium. Record the number of moles to at least four significant figures. Rounding early is not recommended.

2. Examine your mole calculations and identify the least number of moles calculated. Divide all of the mole calculations by the smallest number of moles calculated to simplify the mole:mole ratio. This step may yield whole numbers or very close to whole numbers. If so, these whole numbers serve as the subscripts for the empirical formula.
   a. If the mole:mole ratio contains numbers other than whole numbers you may have to multiply *all* of the moles by the same factor to convert them to whole numbers. Try multiplying by 2 first, then by 3, etc.

   b. For example: If the mole:mole ratio comes out 1: 2.5: 1; multiplying each number in the ratio by 2 will yield the same proportion, but eliminate the ½. The ratio becomes 2: 5: 2. Remember that subscripts must be whole numbers so your calculated mole:mole ratio must be very near whole numbers. Also, remember you must multiply *all* of the calculated moles by the *same* number to keep them proportional.

   c. Watch for numbers that have the following terminal decimal values:
      - $\approx$0.20 (multiply by 5 to yield $\approx$1.0)
      - $\approx$0.25 (multiply by 4 to yield $\approx$1.0)
      - $\approx$0.33 (multiply by 3 to yield $\approx$1.0)
      - $\approx$0.50 (multiply by 2 to yield $\approx$1.0)
      - $\approx$0.67 (multiply by 3 to yield $\approx$ 2.0)
      - $\approx$0.75 (multiply by 4 to yield $\approx$ 3.0)
      - $\approx$0.80 (multiply by 5 to yield $\approx$ 4.0)

3. Write the empirical or molecular formula with proper subscripts and name the compound if asked. (Usually the problem lists the elements in the order they appear in the formula.)

EXAMPLE PROBLEM 1:

Many of the biochemicals 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 during the "fight or flight" response. 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 having a mass of 41.764 grams was found in the photography lab. Analysis of this compound revealed that it was composed of 12.144 grams of sodium, 16.948 grams of sulfur, and the rest of the compound was oxygen. Calculate the empirical formula for this compound and provide its name.

CALCULATING MOLECULAR FORMULAS

It may be necessary for you to calculate the empirical formula first in order to determine the molecular formula. The molecular formula is simply a multiple of the empirical formula.

1. Calculate the empirical formula mass.

2. Determine the factor that the empirical formula will be multiplied by to determine the molecular formula. Simply divide the molecular mass by the empirical formula mass. This should yield a whole number.

3. 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 $180.\frac{\text{g}}{\text{mol}}$ and has an empirical formula of CH_2O. Name this compound.

EXAMPLE PROBLEM 4:

An organic alcohol was quantitatively found to 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/mol, determine the molecular formula and name this alcohol.

USING THE GRAPHING CALCULATOR TO DETERMINE EMPIRICAL FORMULAS

Now that you have mastered the mole concepts involved in performing these calculations, use your graphing calculator to make quick work of the Analysis section. Let's work Example 5 using the TI-83 or TI-83+ graphing calculator.

EXAMPLE PROBLEM 5:

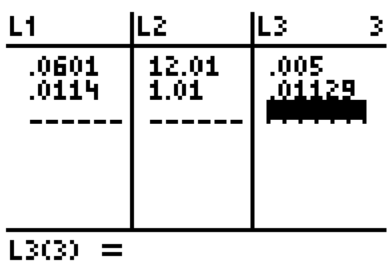
A 71.5 mg sample of an unknown petroleum product was quantitatively analyzed. It was determined that the compound contained 60.1 mg carbon and 11.4 mg hydrogen. Through mass spectrometry, the molecular mass was found to be 114.26 g/mol. What is the molecular formula? Name this molecular compound.

1. Enter the data for each element into L1. It is a good idea to enter it in the order given in the problem so a quick glance back at the problem reminds you which data point matches which element.

2. Since this data is given in milligrams rather than grams, perform a batch transform on L1 by pressing [▲] until the L1 is highlighted at the top of the column. Next, recall that 1,000 g = 1 mg, so you need to divide L1 by 1,000 to transform the data into grams so that you can calculate the number of moles. Do this by pressing [2nd] [2] [÷] [1] [0] [0] [0] [ENTER]. Had the data been given in percent composition or grams, we would skip this step.

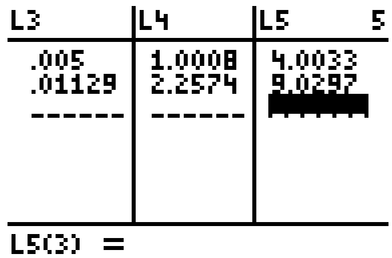
3. Press [►] to go to L2. Enter the atomic masses for each element into L2. Glance back at the problem to ensure that you are entering the correct atomic mass next to the correct data point for each element.

4. Now you are ready to quickly calculate the number of moles of each element present. Press [►] [▲] to highlight L3 at the top of the column. Press [2nd] [1] [÷] [2nd] [2] [ENTER]. At this point your screen should look like this:



5. Simplify the mole:mole ratio. Determine which element has the least number of calculated moles. Press [►] [▲] to highlight L4 at the top of the column. Press [2nd] [3] [÷] [.] [0] [0] [5] [ENTER]. If this generates small whole numbers, you have now determined the subscripts in the empirical formula. This is not the case with this example! We have calculated a 1:2.26 mole:mole ratio.

6. Decide which factor both moles must be multiplied by to generate small whole numbers for our empirical formula subscripts. Press $\boxed{\blacktriangle}$ $\boxed{\blacktriangle}$ to highlight L5 at the top of the column. Press $\boxed{\text{2nd}}$ $\boxed{4}$ $\boxed{\times}$ $\boxed{4}$ $\boxed{\text{ENTER}}$ to convert the 1:2.26 mole ratio to a 4:9 mole ratio. Examining the numbers in L5 makes it easy to see that the empirical formula is C_4H_9. Your screen should look like this:



7. Press $\boxed{\text{2nd}}$ $\boxed{\text{MODE}}$ to quit and return to the home screen. Calculate the empirical formula mass for C_4H_9.

8. Finally, divide the molar mass given (114.26) by the calculated empirical mass (4(12.01) + 9(1.01) = 57.13) to determine the multiplication factor applied to each subscript in the empirical formula in order to determine the molecular formula. In this case it is 2, so you should arrive at a molecular formula of C_8H_{18}. This compound is octane.

Name______________________________________

Period ____________________________________

Simple vs. True
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ANALYSIS

Solve the following problems on this answer page. Be sure to show all work for full credit.

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2. A mysterious white powder was found at a crime scene. It was quantitatively analyzed and its percent composition was determined to be 27.37% sodium, 1.20% hydrogen, 14.30% carbon with the remainder being 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 it was determined 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.