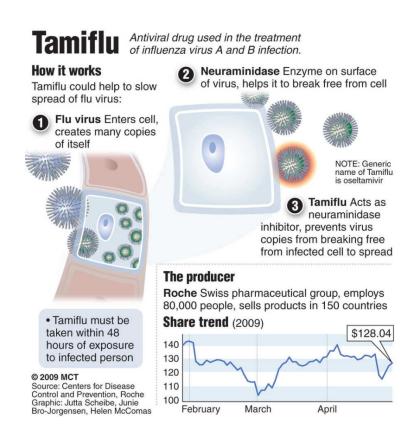
### Lecture Notes Chemistry E-la

### Chapter 3



http://inserbia.info/news/wp-content/uploads/2013/05/Tamiflu.jpg



# **Using The Mole**

**One mole** of something consists of  $6.02 \times 10^{23}$  units of that substance. This number is called **Avogadro's number**. The **molar mass** of a substance is the mass in grams or kilograms of one mole of units of that substance. For us, these 'units' are going to be either atoms or molecules. Let's look at the molar mass of lead and water:

• We can use a balance to weigh out one mole of lead (Pb). If we do this, we find the mass to be:

a. Using this information, write two conversion factors involving Pb:

b. Is there a proper way to write this in terms of numerator and denominator?

- c. How can the periodic table help us find the molar mass of atoms?
- d. How many moles of lead are in 400 g of Pb?

**Bonus:** Use the periodic table to determine the molar mass of one mole of water, then write at least three conversion factors that involve water.

# Putting it all together: Ions, Nomenclature, and Molar Mass

Here is an example of a problem that uses several concepts from all of the lectures we have had so far.

a. How many atoms of carbon are present in 5.732 g of calcium carbonate?

Cacoz Ca: 40.08 3/mole c: 12.01 g/mole 30: 3 x 16 5/mil 100.09 S/mile **Bonus**: A 5.732 g sample of calcium carbonate is heated and 0.64 g carbon dioxide gas is produced. After the carbon dioxide is produced, how many grams of carbon are present in the calcium carbonate that remains? 5.7325 C. CO3 Lose 0.645 CO2 LOST L: 0.64 CO2 x Imole CO2 MASS 6F CALPON IN CaCOZ M CAN

# **Chemical Formulas and Percent Composition**

We have already seen that the **empirical formula** represents the **smallest whole-number ratio** of the various types of atoms in a compound. The **molecular formula** is the exact formula of the molecule involved. Let's look at a new way of representing molecules:

• **Percent composition** is the mass of an element divided by the total mass of the compound:

Percent composition (by mass)

 $\frac{\text{Mass of element}}{\text{Mass of compound}} \times 100\%$ 

General approach to converting between empirical/molecular formula and percent composition for a hypothetical compound:  $A_3B_9X_1$ 

(The molar mass of each element is A=13.71 g/mole, B=22.4 g/mole, and X=52.1 g/mole)

- 1. Assume 1 mole of compound  $A_3B_9X_1$ .
- 2. Determine the number of moles of each element in 1 mole of compound. For our compound above, this would yield:

3 mole A I mole X 9 mole B

3. Determine the mass of each element from the number of moles of each element.

9 mole B x 22.45B = 261.65B

- 4. Add up the total mass of each element to get the total mass of the compound.
- 5. Calculate the % composition :

Percent composition (by mass) =  $\frac{\text{Mass of element (Step 3)}}{\text{Mass of compound (Step 4)}} \times 100\%$ 

## Converting Chemical Formulas to Percent Composition

Solve the problem below using the approach we developed on the previous page for converting the empirical or molecular formula of a compound to the percent composition of each element in that compound.

Bees release the compound  $C_2H_{14}O_2$  when they sting in order to attract other bees to join the attack. An experimental analysis of a pure substance extracted from a banana found that it contained 64.6%  $C_2(10.9\% \text{ H})$ , and 24.6 %  $O_2(10.9\% \text{ H})$ .

Could this substance from the banana be the same compound released by the bees?

# Converting from Percent Composition To Empirical Formula

Now let's do the reverse of what we've done previously and convert the percent composition of a compound to its empirical formula. Once we have the empirical formula, we can then find the molecular formula. Note that in some cases, the empirical formula and molecular formula are identical!

Below is an example of this type of problem:

A molecule isolated from a plant was found to contain 40.92% C, 4.58% H, and 54.50% O by mass. Determine if this substance is Shikimic Acid ( $C_7H_{16}O_5$ ) by finding the empirical formula of the molecule isolated from the plant.

- General approach for converting between percent composition and empirical formula for a hypothetical compound with the following composition: 32% X, 68% Y.

  (The molar mass of X is 15.77 g/mole and the molar mass of Y is 82.24 g/mole.)
- 1. Assume a 100 g sample of a compound.
- 2.Use the percent composition to determine the mass of each element in 100 grams of that compound.

$$32 \text{ Y. } X = \frac{32 \text{ S} \times 100 \text{ N}}{1005} \times 100 \text{ N}.$$

3.Use the mass of each element to determine the number of moles of each element in the 100 g sample.

- 4.Determine which element in the 100 g sample is present in the smallest number of moles. How many moles of this element are there?
- 5. Divide the number of moles of each element in the sample by the number of moles of the element found in step 4 to produce the empirical formula.

6. Each of the elements in an empirical formula must be represented as whole number. If the empirical formula generated in step 5 has one or more elements with a fractional number of moles, multiply the entire empirical formula by a number that will yield the smallest whole number ratios of each of the elements.

# Converting from Percent Composition to Empirical Formula

Using the approach on the previous page for converting from percent composition to the empirical of a compound, solve the problem below:

A molecule isolated from a plant was found to contain 40.92% C, 4.58% H, and 54.50% O by mass. Determine if this substance is Shikimic Acid ( $C_7H_{16}O_5$ ) by finding the empirical formula of the molecule isolated from the plant.

Once we have the empirical formula for a compound how can we determine the molecular formula for that compound?

# Determining the Molecular Formula from the Empirical Formula

As we noted previously, every compound has both a molecular formula and an empirical formula. For some compounds, the empirical formula and the molecular formula will be the same.

General approach for converting an empirical formula to a molecular formula if you are given the molar mass of the molecular formula is as follows:

- 1. Determine the molar mass of the empirical formula
- 2. Divide the molar mass of the molecular formula by the molar mass of the empirical formula.
  - If this ratio is equal to one, then the empirical formula and molecular formula are the same
  - If this ratio is greater than one, then multiply the empirical formula by this ratio to produce the molecular formula for this compound.

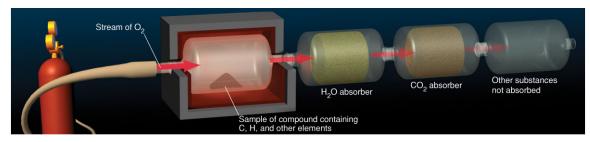
You found the empirical formula for a molecule isolated from a plant. The molar mass of the molecule is 175.14 g/mol.

a. Using the information above and the empirical formula you found on the previous page, determine the molecular formula of the molecule isolated from the plant.

#### **Experiments Used to Determine Empirical Formulas**

Combustion Analysis is the name of an experiment that can be used to determine the empirical formula for any compound that can be combusted in air. We are going to look at using this experiment for compounds that have at least the elements carbon and hydrogen.

When any compound containing carbon and hydrogen is completely combusted, carbon dioxide and water are produced as products. If the mass of CO<sub>2</sub> and H<sub>2</sub>O produced are measured, the **empirical formula of the original compound** can be determined.



General approach to using the experimental results from a combustion analysis experiment to determine the empirical formula for a combusted compound.

- 1.Using mass of  $CO_2$  produced in experiment  $\rightarrow$  determine moles of C atoms present in combusted compound
- 2.Using mass of H<sub>2</sub>O produced in experiment → determine moles of H atoms present in combusted compound
- 3. Gather any remaining information to determine the empirical formula.
- •If the combusted compound contains only C and H → determine the empirical formula by finding the lowest whole number mole ratio of elements in the combusted compound.
- •If the combusted compound contains C, H, and other elements  $\rightarrow$  you will need to use additional pieces of information to determine the empirical formula of the compound.
- •If an additional element like O is present and you know the total mass of the combusted compound • use the total mass to find the moles of oxygen present.

Total mass of compound - (Mass of C + Mass of H) = Mass of O

Using mass of O in combusted compound → determine moles of O atoms present in combusted compound

Now, determine the empirical formula by finding the lowest whole number mole ratio of elements in the combusted compound.

# Using Combustion Analysis to Determine the Empirical Formula for a Compound

Use the general approach on the previous page to solve problem below.

a. Compound X contains only carbon, hydrogen, and oxygen. When \$1.000-gram sample of Compound X is subjected to combustion analysis, 2.432 grams of CO<sub>2</sub> and 0.574 grams of H<sub>2</sub>O are produced. Determine the empirical formula of Compound X.



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#### A Short Enantioselective Pathway for the Synthesis of the Anti-Influenza Neuramidase Inhibitor Oseltamivir from 1,3-Butadiene and Acrylic Acid

Ying-Yeung Yeung, Sungwoo Hong, and E. J. Corey\*

Department of Chemistry and Chemical Biology, Harvard University, Cambridge, Massachusetts 02138

Received March 9, 2006; E-mail; corev@chemistrv.harvard.edu

The recent emergence of the avian virus H5N1 raises the possibility of a pandemic wave of life-threatening flu that requires prompt action.\(^1\) A four-pronged effort to avert widespread disease is now underway that consists of the following components: (1) worldwide surveillance of both wild and domesticated birds with quick culling of the latter, (2) development of recombinant vaccines against the H5N1 virus and its mutated forms whose production can be scaled up rapidly,\(^2\) (3) procedures for quarantine, and (4) ramped up production of the orally effective, synthetic neuramidase inhibitor oseltamivir phosphate (Tamiflu) (1).\(^3\) This paper describes a total synthesis of 1 that would appear to have a number of advantages over existing processes and the potential to increase the rate of production.

Heroic efforts by synthetic chemists at Gilead Sciences, Inc.<sup>4</sup> and F. Hoffman—La Roche, Ltd.<sup>5</sup> have resulted in the development of several synthetic pathways to 1, culminating in the current production method.<sup>5</sup> That process falls short of the ideal for several reasons: (1) the starting point in the synthesis is either (-)-shikimic or (-)-quinic acid, which are complex relatively expensive and of limited availability, and (2) two steps involve potentially hazardous

and explosive azide-containing intermediates. The route described herein has been used for the synthesis of oseltamivir and also its enantiomer.

The synthesis of 1 is summarized in Scheme 1. We have previously described the reaction of butadiene with trifluoroethyl

#### Scheme 1

## **Balancing Chemical Equations**

Atoms are conserved in a chemical reaction. Whenever you see an equation, you should ask yourself whether it is balanced by making sure the same number and type of atoms appear on each side of the reaction arrow. Look at the example below

$$3 A_2 R + 6 D \rightarrow 6 AD + 3 R$$

Note how there are the same number of A, D, and R atoms on each side of the arrow

a. Write the complete, balanced chemical equation for each of the following reactions:

$$C_4H_{10} + \frac{13}{2}O_2 \rightarrow 4CO_2 + 5H_2O$$

**Bonus:** Solid iron (III) sulfide reacts with gaseous hydrogen chloride to form solid iron (III) chloride and hydrogen sulfide gas. Write the complete, balanced chemical equation for this process.

# **Quantifying Chemical Reactions: Determining Amounts of Reactants Used or Products Produced**

If you entered Harvard as a freshman in the fall of 1919, the reaction between copper and oxygen to give copper (II) oxide would be one of the first experiments you performed.

Suppose you go into the lab with 1.123 g of copper metal. What mass of copper (II) oxide will be produced if **all** of the copper reacts with oxygen?

a. Write a complete, balanced chemical equation for this reaction.

b. Determine the number of moles of copper metal present at the start of the reaction.

c. Find the ratio between the number of moles of copper that react and the number of moles of copper oxide that are formed? (Hint: The balanced chemical reaction tells us this

d. This ratio is a conversion factor! Use this conversion factor to find the number of moles of copper oxide produced.

e. What assumption did we make about the amount of oxygen present in solving this problem? problem? Unlim Hed Amount of Oz

**Bonus:** Determine the amount of oxygen consumed in this reaction.

#### **Reaction Yield**

Often, chemical reactions will not produce as much product as is theoretically possible. You will find this to be the case in the lab when you react copper with oxygen.

Previously, we determined the **theoretical yield** of copper oxide if 1.123 grams of Cu reacts with oxygen to produce copper oxide. In practice, not all of the copper will react!

Let's see why...

a. Suppose I gave you a large block of copper metal and the same mass of copper chopped up into small pieces. Which sample would you expect to produce more copper oxide product during a reaction with the unlimited amount of oxygen in the air? Circle your choice, then explain your answer.



b. The **percent yield** of a reaction can be used to determine the actual yield of product formed in a particular experiment.

ActualYield

ActualYield

1000/

Suppose the percent yield of copper (II) oxide for the reaction of copper with oxygen is only 13%. What mass of copper (II) oxide will be produced in our reaction of 1.123 grams of Cu?

### **Activity 3.09 - Understanding Limiting Reactants**

Let's now consider a different case, where we do not have an unlimited supply the other reactant(s).

What if we were able to obtain 100% yield from the reaction, but were limited in the amount of product produced because one of the reactants is completely used up before the other reactants.

Consider the chemical reaction where  $NO_2$  is produced by reacting NO with  $O_2$ .

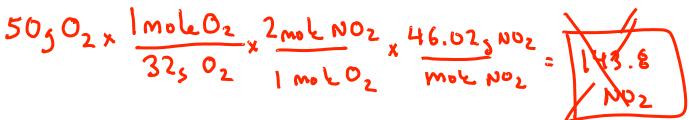
If 50 grams of NO is reacted with 50 grams of  $O_2$ , how can we determine how much nitrogen dioxide is produced? Follow the approach below to determine how much nitrogen dioxide is made and assume the reaction yield is 100%.

Step 1: Write the complete, balanced chemical reaction.

$$2NO + O_2 \rightarrow 2NO_2$$

Step 2: Determine the amount of product produced if 50 g of NO reacts *completely* with an unlimited amount of oxygen:

Step 3: Determine the amount of product produced if 50 g of O<sub>2</sub> reacts *completely* with an unlimited amount of NO:



Step 4: Compare the amount of product produced in Step 2 and Step 3. The reactant that produces the least amount of product is the limiting reactant!

### A New Type of Problem Involving Mixtures

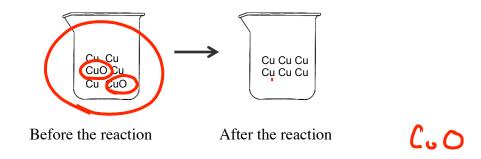
To really test our knowledge of chemical reactions, we can work a new kind of problem. A mixture problem!

You have a mixture of Cu and CuO which weighs a total of 1.227 grams. This mixture is placed inside a container. Complete reduction of this mixture yields 1.123 grams of Cu. Determine the mass of Cu and CuO in the original mixture.

One way of writing the reduction reaction for CuO is below:

$$CuO \rightarrow Cu + \frac{1}{2}O_2$$

First, let's create a drawing to represent what is happening in the reaction. Drawn on the diagram below is what the container contents might look like before and after the reaction. Note the oxygen is not in the container after the reaction!



a. Determine the mass of oxygen atoms that were bound to the CuO before the reduction

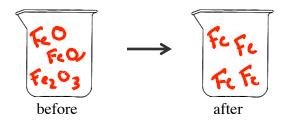
c. Using this mass of oxygen atoms determine the amount of CuO in the original sample and then the amount of Cu in the original sample.

### **Putting it together: Mixtures**

Now, let's see how we might combine the topics we've already discussed to make a mixture problem slightly more challenging.

You are given a 10.00 gram mixture of FeO and Fe<sub>2</sub>O<sub>3</sub>. This mixture is placed inside a container. Complete reduction of this mixture yields 7.46 grams of pure iron. Calculate the mass of each iron oxide in the original sample.

a.Draw a picture representing the contents of the container before and after the reaction.



- Assign the variable of x to the mass of the FeO and the variable of y to the mass of  $Fe_2O_3$ .
- b. Using these variables write an expression for the total mass of FeO and Fe<sub>2</sub>O<sub>3</sub> mixture before it was reduced.

• One way to represent the reduction reactions that are occur in the container is to use the reactions written below

FeO 
$$\rightarrow$$
 Fe +  $\frac{1}{2}$  O<sub>2</sub>  
Fe<sub>2</sub>O<sub>3</sub>  $\rightarrow$  2Fe +  $\frac{3}{2}$  O<sub>2</sub>

c. Using these reactions and the variables assigned above write an equation that equates the amount of pure iron produced from the reduction of FeO and the amount of pure iron produced by the reduction of  $Fe_2O_3$  to the total amount of pure iron produced from both reduction reactions.

# **Stoichiometry of Mixtures (continued)**

$$0.777x + 0.699y = 7.46$$

$$y = 10 - x = y = 10 - 6.026 = \sqrt{3.97 = y}$$

$$Fe_{2}O_{3}$$