

EXAMPLE 3.9

Calculating the Percentages of C and H by Combustion

Acetic acid contains only C, H, and O. A 4.24-mg sample of acetic acid is completely burned. It gives 6.21 mg of carbon dioxide and 2.54 mg of water. What is the mass percentage of each element in acetic acid?



PROBLEM STRATEGY

You first convert the mass of CO_2 to moles of CO_2 . Then you convert this to moles of C, noting that 1 mol C produces 1 mol CO_2 . Finally, you convert to mass of C. Similarly, you convert the mass of H_2O to mol H_2O , then to mol H, and finally to mass of H. (Remember that 1 mol H_2O produces 2 mol H.) Once you have the masses of C and H, you can calculate the mass percentages. Subtract from 100% to get % O.

SOLUTION

Following is the calculation of grams C:

$$6.21 \times 10^{-3} \text{ g CO}_2 \times \frac{1 \text{ mol CO}_2}{44.0 \text{ g CO}_2} \times \frac{1 \text{ mol C}}{1 \text{ mol CO}_2} \times \frac{12.0 \text{ g C}}{1 \text{ mol C}} \\ = 1.69 \times 10^{-3} \text{ g C (or 1.69 mg C)}$$

For hydrogen, you note that 1 mol H_2O yields 2 mol H, so you write

$$2.54 \times 10^{-3} \text{ g H}_2\text{O} \times \frac{1 \text{ mol H}_2\text{O}}{18.0 \text{ g H}_2\text{O}} \times \frac{2 \text{ mol H}}{1 \text{ mol H}_2\text{O}} \times \frac{1.01 \text{ g H}}{1 \text{ mol H}} \\ = 2.85 \times 10^{-4} \text{ g H (or 0.285 mg H)}$$

You can now calculate the mass percentages of C and H in acetic acid.

$$\text{Mass \% C} = \frac{1.69 \text{ mg}}{4.24 \text{ mg}} \times 100\% = 39.9\%$$

$$\text{Mass \% H} = \frac{0.285 \text{ mg}}{4.24 \text{ mg}} \times 100\% = 6.72\%$$

You find the mass percentage of oxygen by subtracting the sum of these percentages from 100%:

$$\text{Mass \% O} = 100\% - (39.9\% + 6.72\%) = 53.4\%$$

Thus, the percentage composition of acetic acid is **39.9% C, 6.7% H, and 53.4% O**.

EXERCISE 3.9

A 3.87-mg sample of ascorbic acid (vitamin C) gives 5.80 mg CO_2 and 1.58 mg H_2O on combustion. What is the percentage composition of this compound (the mass percentage of each element)? Ascorbic acid contains only C, H, and O.

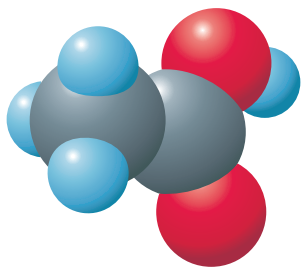
See Problems 3.57 and 3.58.

CONCEPT CHECK 3.2



You perform combustion analysis on a compound that contains only C and H.

- Considering the fact that the combustion products CO_2 and H_2O are colorless, how can you tell if some of the product got trapped in the CuO pellets (see Figure 3.6)?
- Would your calculated results of mass percentage of C and H be affected if some of the combustion products got trapped in the CuO pellets? If your answer is yes, how might your results differ from the expected values for the compound?

**Figure 3.10****Molecular model of acetic acid**

The hydrogen atom (blue atom at the top right) attached to the oxygen atom (red atom) is easily lost, so it is acidic. The three hydrogen atoms attached to the carbon atom (black atom at the left) are not acidic.

summing the atomic weights of the atoms in the empirical formula. For any molecular compound, you can write

$$\text{Molecular weight} = n \times \text{empirical formula weight}$$

where n is the number of empirical formula units in the molecule. You get the molecular formula by multiplying the subscripts of the empirical formula by n , which you calculate from the equation

$$n = \frac{\text{molecular weight}}{\text{empirical formula weight}}$$

Once you determine the empirical formula for a compound, you can calculate its empirical formula weight. If you have an experimental determination of its molecular weight, you can calculate n and then the molecular formula. The next example illustrates how you use percentage composition and molecular weight to determine the molecular formula of acetic acid.

EXAMPLE 3.12**Determining the Molecular Formula from Percentage Composition and Molecular Weight**

In Example 3.9, we found the percentage composition of acetic acid to be 39.9% C, 6.7% H, and 53.4% O. Determine the empirical formula. The molecular weight of acetic acid was determined by experiment to be 60.0 amu. What is its molecular formula?

SOLUTION

A sample of 100.0 g of acetic acid contains 39.9 g C, 6.7 g H, and 53.4 g O. Converting these masses to moles gives 3.33 mol C, 6.6 mol H, and 3.34 mol O. Dividing the mole numbers by the smallest one gives 1.00 for C, 2.0 for H, and 1.00 for O. **The empirical formula of acetic acid is CH₂O.** (You may have noted that the percentage composition of acetic acid is, within experimental error, the same as that of formaldehyde—see Example 3.7—so they must have the same empirical formula.) The empirical formula weight is 30.0 amu. Dividing the empirical formula weight into the molecular weight gives the number by which the subscripts in CH₂O must be multiplied.

$$n = \frac{\text{molecular weight}}{\text{empirical formula weight}} = \frac{60.0 \text{ amu}}{30.0 \text{ amu}} = 2.00$$

The molecular formula of acetic acid is (CH₂O)₂, or C₂H₄O₂.

EXERCISE 3.12

The percentage composition of acetaldehyde is 54.5% C, 9.2% H, and 36.3% O, and its molecular weight is 44 amu. Obtain the molecular formula of acetaldehyde.

See Problems 3.67, 3.68, 3.69, and 3.70.

The formula of acetic acid is often written HC₂H₃O₂ to indicate that one of the hydrogen atoms is acidic (lost easily) while the other three are not (Figure 3.10). Now that you know the formulas of acetic acid and acetaldehyde (determined from the data

CHEMICAL FORMULAS

- Formulas give information about the type, the number, and arrangement of atoms in a substance
- Two important type of formulas will be discussed and compared:

MOLECULAR FORMULAS	EMPIRICAL FORMULAS (Simplest Formulas)	
can be written for molecular compounds only	can be written for both molecular and ionic compounds	
- indicate the number of atoms of each kind in a molecule - are multiples of empirical formulas	indicate the smallest whole number ratio between the atoms or ions of a substance (smallest whole number subscripts)	
		Multiplier
H ₂ O ₂ (hydrogen peroxide)	HO	2
H ₂ O	H ₂ O	1
C ₂ H ₂ (acetylene)	CH	2
C ₆ H ₆ (benzene)	CH	6
C ₆ H ₁₂ O ₆ (glucose)	CH ₂ O	6
C ₆ H ₁₂ (cyclohexane)	CH ₂	6
C ₆ H ₄ Cl ₂	C ₃ H ₂ Cl	2
Does not exist for an Ionic Compound	NaCl	--
Does not exist for an ionic compound	SnO ₂	--

Calculating the Empirical (Simplest Formula)

Information Required: - Percentage Composition by Mass, or
- Composition by weight

Example:

Tin (Sn) reacts with oxygen (O) to form an oxide of tin (Sn_aO_b), which contains 0.9913 g Sn and 0.2729 g O.

What is the Empirical Formula of the oxide ?

(that is: a = ? b = ?)

Step 1: MASS \longrightarrow MOLE

$$? \text{ moles Sn} = \cancel{0.9913 \text{ g Sn}} \times \frac{1 \text{ mole Sn}}{\cancel{118.71 \text{ g Sn}}} = 0.008351 \text{ moles Sn atoms}$$

$$? \text{ moles O} = \cancel{0.2729 \text{ g O}} \times \frac{1 \text{ mole O}}{\cancel{16.00 \text{ g O}}} = 0.01706 \text{ moles O atoms}$$

Step 2: DIVIDE BY SMALL

$$\text{Relative number of O atoms} = \frac{0.01706 \text{ moles O}}{0.008351 \text{ moles Sn}} = 2.043$$

$$\text{Relative number of Sn atoms} = \frac{0.008351 \text{ moles Sn}}{0.008351 \text{ moles Sn}} = 1.000$$

Empirical Formula: $\text{Sn}_{1.000}\text{O}_{2.043} \longrightarrow \text{SnO}_2$
(includes experimental error)

Sample Problem # 1

Arsenic (As) reacts with oxygen (O) to form a compound that is 75.7 % As and 24.3 % O by mass.

What is the empirical formula of this oxide ?

Step 1: PERCENT → MASS

	75.7 % As	24.3% O	
	↓	↓	
Assume 100 g compound →	75.7 g As	24.3 g O	

Step 2: MASS → MOLE

$$? \text{ moles As} = \frac{75.7 \text{ g As}}{74.92 \text{ g As}} \times \frac{1 \text{ mole As}}{1} = 1.01 \text{ moles As atoms}$$

$$? \text{ moles O} = \frac{24.3 \text{ g O}}{16.00 \text{ g O}} \times \frac{1 \text{ mole O}}{1} = 1.52 \text{ moles O atoms}$$
Step 3: DIVIDE BY SMALL

$$\text{Relative number of O atoms} = \frac{1.52 \text{ moles O}}{1.01 \text{ moles As}} = 1.50$$

$$\text{Relative number of As atoms} = \frac{1.01 \text{ moles As}}{1.01 \text{ moles As}} = 1.00$$

Empirical Formula: **As_{1.00}O_{1.50} ??????????**
 (subscripts must be whole numbers)

Step 4: MULTIPLY 'TIL WHOLE:

A Simple Rhyme for a Simple Formula
(to be remembered)

1. **Percent to Mass**
2. **Mass to Mole**
3. **Divide by small**
4. **Multiply 'til Whole**

Sample Problem # 1

A sample of Freon contains 0.423 g C, 2.50 g Cl, and 1.34 g F. What is the Empirical Formula of Freon?

1. Percent to Mass

This step may be skipped since masses are already given:

0.423 g C

2.50 g Cl

1.34 g F.

2. Mass to Mole

? moles C =

? moles Cl =

? moles F =

3. Divide by small

C =

Cl =

F =

Empirical Formula: _____

Sample Problem 1

The empirical formula for benzene is CH. The molecular mass of benzene is 78 amu. What is the molecular formula of benzene?

Empirical Formula Mass of CH is:

$$\begin{array}{rcl} 1 \text{ C} & = & 1 \times 12 \text{ amu} & = & 12 \text{ amu} + \\ 1 \text{ H} & = & 1 \times 1 \text{ amu} & = & 1 \text{ amu} \\ & & & & \hline & & & & 13 \text{ amu} \end{array}$$

Molecular Formula: $(\text{CH})_n$ $n = ?$

$$n = \frac{\text{Molecular Mass}}{\text{Empirical Formula Mass}} = \frac{78 \text{ amu}}{13 \text{ amu}} = 6$$

Sample Problem 2:

A compound whose empirical formula is $\text{C}_3\text{H}_2\text{Cl}$ has a Molecular Mass of 147.0 amu. What is the Molecular Formula ?

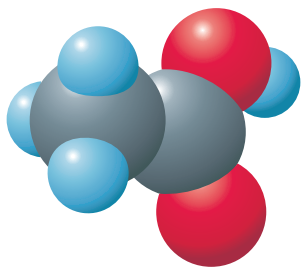
Empirical Formula Mass of $\text{C}_3\text{H}_2\text{Cl}$ is:

$$\begin{array}{rcl} 3 \text{ C} & = & 3 \times 12.0 \text{ amu} & = & 36.0 \text{ amu} + \\ 2 \text{ H} & = & 2 \times 1.0 \text{ amu} & = & 2.0 \text{ amu} \\ 1 \text{ Cl} & = & 1 \times 35.5 \text{ amu} & = & 35.5 \text{ amu} \\ & & & & \hline & & & & 73.5 \text{ amu} \end{array}$$

Molecular Formula: $(\text{C}_3\text{H}_2\text{Cl})_n$ $n = ?$

$$n = \frac{\text{Molecular Mass}}{\text{Empirical Formula Mass}} = \frac{147 \text{ amu}}{73.5 \text{ amu}} = 2$$



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SOLUTION

A sample of 100.0 g of acetic acid contains 39.9 g C, 6.7 g H, and 53.4 g O. Converting these masses to moles gives 3.33 mol C, 6.6 mol H, and 3.34 mol O. Dividing the mole numbers by the smallest one gives 1.00 for C, 2.0 for H, and 1.00 for O. **The empirical formula of acetic acid is CH₂O.** (You may have noted that the percentage composition of acetic acid is, within experimental error, the same as that of formaldehyde—see Example 3.7—so they must have the same empirical formula.) The empirical formula weight is 30.0 amu. Dividing the empirical formula weight into the molecular weight gives the number by which the subscripts in CH₂O must be multiplied.

$$n = \frac{\text{molecular weight}}{\text{empirical formula weight}} = \frac{60.0 \text{ amu}}{30.0 \text{ amu}} = 2.00$$

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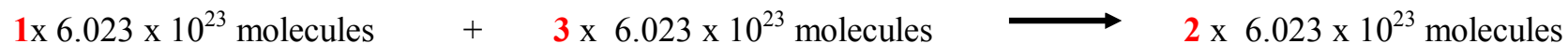
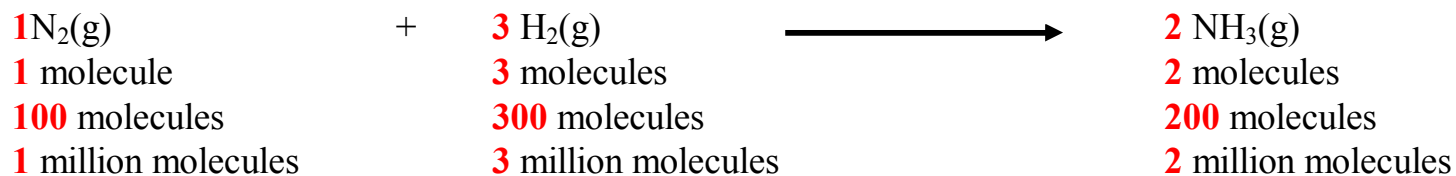
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STOICHIOMETRY
QUANTITATIVE RELATIONS IN CHEMICAL REACTIONS

Stoichiometry: calculations of the quantities of reactants and products involved in a chemical reaction.

- Based on:
1. Balanced chemical equation (mole ratio)
 2. Relationship between mass and moles
 3. Proportional thinking

Consider the industrial process by which NH_3 is obtained:

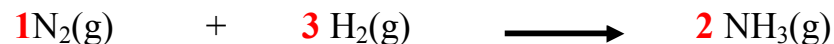


THIS IS THE MOLE RATIO BETWEEN REACTANTS AND PRODUCTS

Note: The mole ratio is given by the coefficients of the balanced chemical equation.

Example 1:

How many moles of nitrogen will react with 2.4 moles of hydrogen ?



$$? \text{ moles N}_2 = 2.4 \text{ moles H}_2 \times \frac{1 \text{ mole N}_2}{3 \text{ moles H}_2} = 0.80 \text{ moles N}_2$$

Mole Ratio

Example 2:

How many moles of NH₃ can be produced from 32 moles of hydrogen ? (Assume there is plenty nitrogen available)



$$? \text{ moles NH}_3 = 32 \text{ moles H}_2 \times \frac{2 \text{ moles NH}_3}{3 \text{ moles H}_2} = \quad \text{moles NH}_3$$

Example 3:

Butane, C₄H₁₀, burns with the oxygen in air to give carbon dioxide and water. How many moles of carbon dioxide are produced from 0.15 moles C₄H₁₀

(Assume sufficient amount of oxygen is available)



$$? \text{ moles CO}_2 = 0.15 \text{ mole C}_4\text{H}_{10} \times \frac{8 \text{ moles CO}_2}{2 \text{ moles C}_4\text{H}_{10}} = \quad \text{mole CO}_2$$

- Quantities of reactants and products may also be expressed in grams.
- The reasoning is similar, but the conversion from the given quantity to the quantity we are looking for should be done through the mole ratio.

Mass \longrightarrow Moles

Consider the following balanced equation:



How many **moles of HClO₃** are produced from **14.3 g of ClO₂**? (Assume excess amount of water)

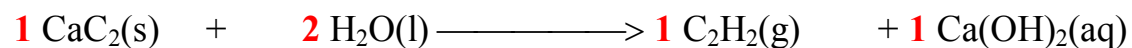
$$? \text{ mole HClO}_3 = 14.3 \text{ g-ClO}_2 \times \frac{1 \text{ mole-ClO}_2}{67.45 \text{ g-ClO}_2} \times \frac{5 \text{ mole HClO}_3}{6 \text{ mole-ClO}_2} = 0.177 \text{ mole HClO}_3$$

Example 1:

How many moles of water are required to produce 30.0 g of HClO₃ ?

Moles \longrightarrow **Mass**

Acetylene gas, C_2H_2 , is produced in a reaction between calcium carbide, CaC_2 , and water, according to the following equation:

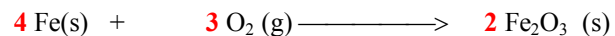


How many **grams of C_2H_2** can be obtained from **0.500 mole CaC_2** ? (Assume an excess of water)

$$? \text{ g } C_2H_2 = 0.500 \text{ mole } CaC_2 \times \frac{1 \text{ mole } C_2H_2}{1 \text{ mole } CaC_2} \times \frac{26.04 \text{ g } C_2H_2}{1 \text{ mole } C_2H_2} = 13.0 \text{ g } C_2H_2$$

Example 2:

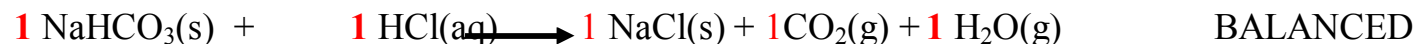
How many grams of iron are required to produce 3.90 mol of Fe_2O_3 as shown below:



Mass → Mass

A sample of solid sodium hydrogen carbonate is reacted with excess hydrochloric acid and produces a white solid residue (sodium chloride) and two gaseous products (carbon dioxide and water vapor).

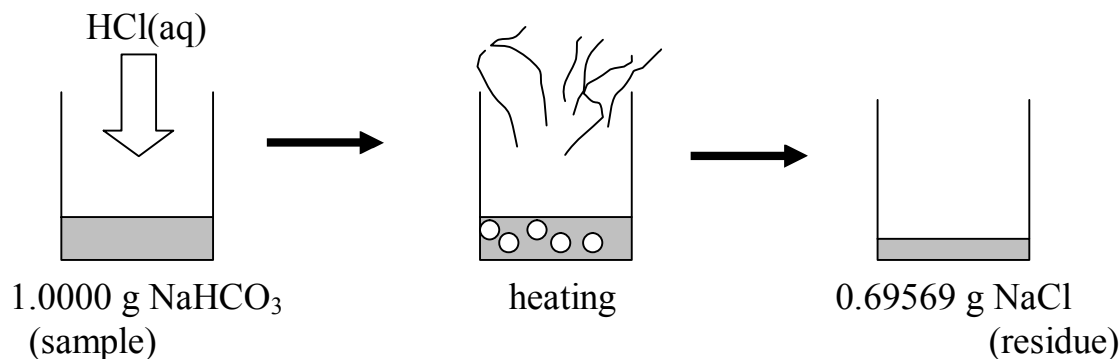
1. Write a balanced chemical equation for this reaction. Include state designations.



2. Calculate the **mass of solid residue (NaCl)** obtained from **1.0000 g NaHCO₃**

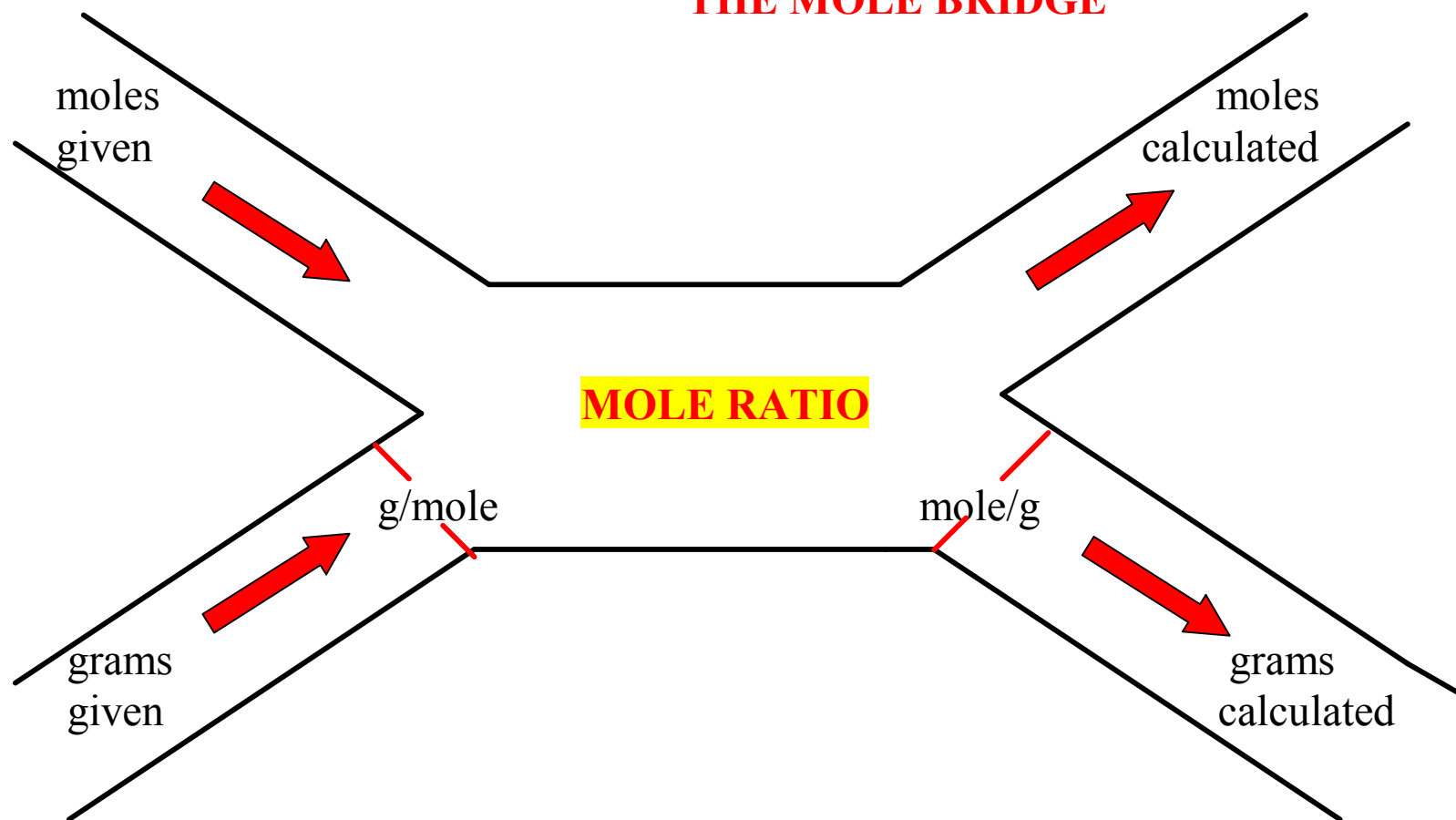
$$? \text{ g NaCl} = 1.0000 \text{ g NaHCO}_3 \times \frac{1 \text{ mole NaHCO}_3}{84.007 \text{ g NaHCO}_3} \times \frac{1 \text{ mole NaCl}}{1 \text{ mole NaHCO}_3} \times \frac{58.443 \text{ g NaCl}}{1 \text{ mole NaCl}} = 0.69569 \text{ g NaCl}$$

3. How much is the total mass of the gaseous products (**CO₂ + H₂O**) given off?



$$\text{Mass of } (\text{CO}_2 + \text{H}_2\text{O}) \text{ given off} = 1.0000 \text{ g NaHCO}_3 - 0.69569 \text{ g NaCl} = 0.3043 \text{ g}$$

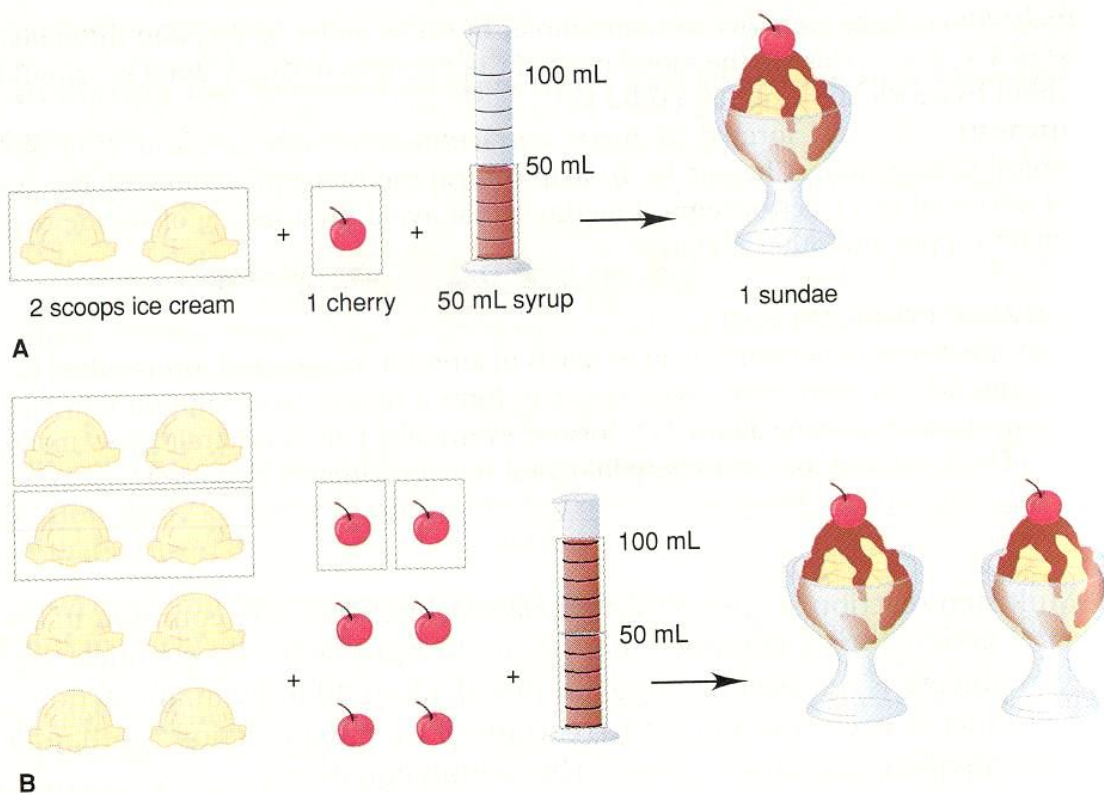
SUMMARY OF STOICHIOMETRIC CALCULATIONS
THE MOLE BRIDGE



ALL STOICHIOMETRIC CALCULATIONS ARE BASED ON THE MOLE RATIO

LIMITING REACTANT

- When **2 or more reactants** are combined in **non-stoichiometric** ratios, the amount of **product** produced is **limited** by the reactant that is **not in excess (limiting reactant)**.

Analogy:

The number of sundaes possible is **limited** by the amount of syrup, the **limiting reactant**.

Limiting Reactant (Reagent) Problems always involve 2 steps:

1. **Identify the Limiting Reactant (LR)**

- convert all masses to moles
- compare actual mole ratio to mole ratio given by the the balanced chemical equation

OR

- calculate the number of moles obtained from each reactant in turn.
- The reactant that gives the smaller amount of product is the Limiting R.eactant.

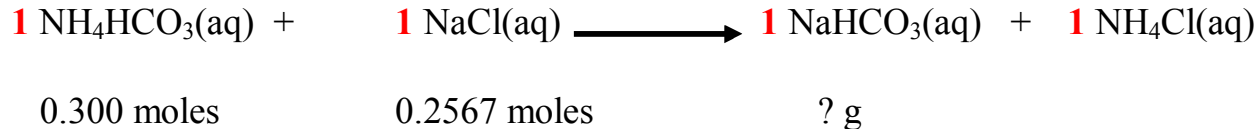
2. **Calculate the amount of product obtained from the Limiting Reactant**

Example 1

Sodium hydrogen carbonate is prepared from NaCl and ammonium hydrogen carbonate, according to the equation:



If 0.300 moles of NH_4HCO_3 are reacted with 0.2567 moles of NaCl, how many grams of NaHCO_3 are obtained ?

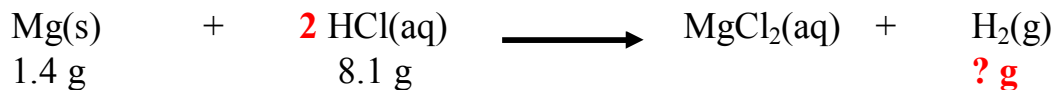


L.R.

$$\begin{aligned} ? \text{ g NaHCO}_3 &= 0.2567 \text{ moles NaCl} \times \frac{1 \text{ mole NaHCO}_3}{1 \text{ mole NaCl}} \times \frac{84.01 \text{ g NaHCO}_3}{1 \text{ mole NaHCO}_3} \\ &= \mathbf{21.57 \text{ g NaHCO}_3} \end{aligned}$$

Example 2

A 1.4 g sample of magnesium is treated with 8.1 g of hydrochloric acid to produce magnesium chloride and hydrogen gas. How many grams of hydrogen are produced ?



Change masses of reactants in moles:



$$\begin{array}{c} \boxed{\begin{array}{c} 1 \text{ mole} \\ 1.4 \text{ g} \times \frac{\quad}{24.31 \text{ g}} \end{array}} \end{array}$$

0.0576 moles

L.R.

requires

$$\boxed{\begin{array}{c} 1 \text{ mole} \\ 8.1 \text{ g} \times \frac{\quad}{36.46 \text{ g}} \end{array}}$$

0.222 moles

2 x 0.0576 moles HCl = 0.115 moles HCl

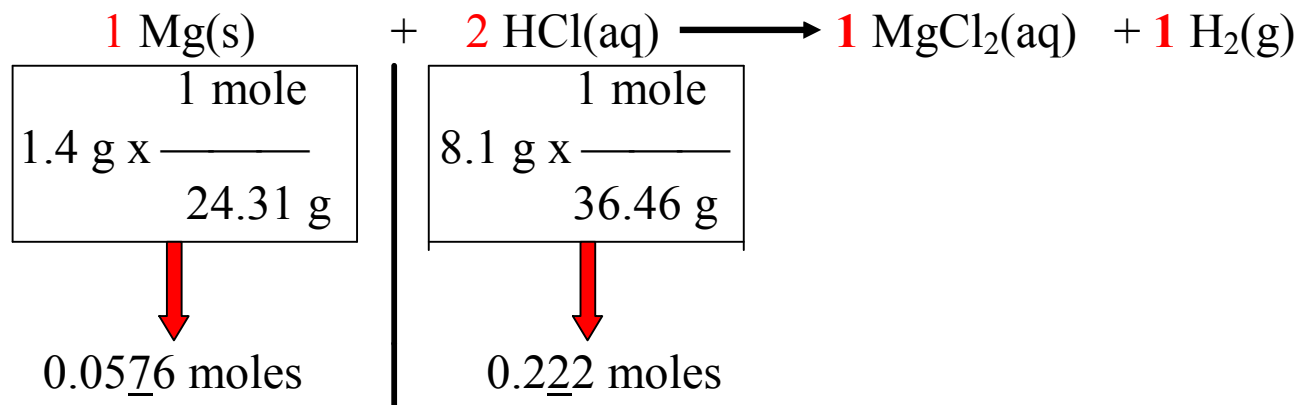
(0.222 moles HCl) available

HCl is an excess!

$$? \text{ g H}_2 = 0.0576 \text{ moles Mg} \times \frac{1 \text{ mole H}_2}{1 \text{ mole Mg}} \times \frac{2.02 \text{ g H}_2}{1 \text{ mole H}_2} = \mathbf{0.12 \text{ g H}_2}$$

L.R.

Solution recommended by textbook:



Calculate the number of moles obtained from each reactant in turn. The reactant that gives the smaller amount of product is the Limiting Reactant.

$$? \text{ g H}_2 = \text{0.222 moles HCl} \times \frac{1 \text{ mole H}_2}{2 \text{ moles HCl}} \times \frac{2.02 \text{ g H}_2}{1 \text{ mole H}_2} = \text{0.22 g H}_2$$

$$? \text{ g H}_2 = \text{0.0576 moles Mg} \times \frac{1 \text{ mole H}_2}{1 \text{ mole Mg}} \times \frac{2.02 \text{ g H}_2}{1 \text{ mole H}_2} = \text{0.12 g H}_2$$

smaller !
(correct answer)

Since Mg produces the smaller amount of product, Mg is the L.R.

THE YIELD CONCEPT

- Quantities of product calculated represent the maximum amount obtainable (100 % yield)
- Most chemical reactions do not give 100 % yield of product because of:
 - side reactions (unwanted reactions)
 - reversible reactions (reactants \longleftarrow products)
 - losses in handling and transferring

$$\text{Percent Yield} = \frac{\text{Actual Yield}}{\text{Theoretical Yield}} \times 100$$

Actual Yield: Amount of product actually obtained (experimental)

Theoretical Yield: Maximum amount of product obtainable (calculated from equation)

Example 1

A 35.0 g sample of calcium hydroxide is reacted with excess phosphoric acid, according to the following balanced chemical equation:



(a) How many grams of calcium phosphate can be produced ?

$$? \text{ g Ca}_3(\text{PO}_4)_2 = 35.0 \text{ g Ca(OH)}_2 \times \frac{1 \text{ mole Ca(OH)}_2}{74.10 \text{ g Ca(OH)}_2} \times \frac{1 \text{ mole Ca}_3(\text{PO}_4)_2}{3 \text{ mole Ca(OH)}_2} \times \frac{310.3 \text{ g Ca}_3(\text{PO}_4)_2}{1 \text{ mole Ca}_3(\text{PO}_4)_2} = 48.9 \text{ g Ca}_3(\text{PO}_4)_2$$

(b) If **45.2 grams** of calcium phosphate are actually obtained in a **laboratory experiment**, what is the percent yield ?

$$\text{Percent Yield} = \frac{\text{Actual Yield}}{\text{Theoretical Yield}} \times 100 = \frac{45.2 \text{ g}}{48.9 \text{ g}} \times 100 = 92.4 \%$$

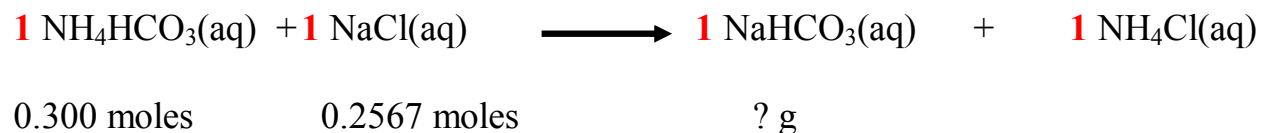
Example 2

Sodium hydrogen carbonate is prepared from NaCl and ammonium hydrogen carbonate, according to the equation:



If 0.300 moles of NH_4HCO_3 are reacted with 0.2567 moles of NaCl, and 10.45 g of NaHCO_3 are obtained, what is the percent yield?

1. First calculate the maximum amount obtainable (theoretical yield) from the given quantities (theoretical yield)



L.R.

$$? \text{ g NaHCO}_3 = \mathbf{0.2567 \text{ moles NaCl}} \times \frac{\mathbf{1 \text{ mole NaHCO}_3}}{\mathbf{1 \text{ mole NaCl}}} \times \frac{84.01 \text{ g NaHCO}_3}{1 \text{ mole NaHCO}_3} = \mathbf{21.57 \text{ g NaHCO}_3 \text{ (theoretical yield)}}$$

2. Second, calculate % yield from actual and theoretical yield

$$\text{Percent Yield} = \frac{\text{Actual Yield}}{\text{Theoretical Yield}} \times 100 = \frac{10.45 \text{ g}}{21.57 \text{ g}} \times 100 = \mathbf{48.45 \%}$$