Chapter 3. Mass Relationships in Chemical Reactions

Atomic & Molecular Masses (Sections 3.1, 3.3) Avogadro's Number, the Mole and Molar Mass (Section 3.2) The Mass Spectrometer (Section 3.4) Percent Composition & Chemical Formulas (Sections 3.5 – 3.6) Chemical Reactions and Chemical Equations (Section 3.7) Amounts of Reactants and Products (Section 3.8) Limiting Reagents & Reaction Yield (Sections 3.9 - 3.10)

SUMMARY

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Atomic & Molecular Masses (Section 3.1)

The Atomic Mass Scale. The masses of individual atoms are too small to be measured with a balance; but the *relative* masses of the atoms of different elements can be measured. For instance, it is possible to determine that an atom of ${}^{4}_{2}$ He is very close to 1/3 the mass of an atom of ${}^{12}_{6}$ C. This is the basis of the atomic mass scale. By international agreement, an atom of carbon-12 is assigned a mass of exactly 12 atomic mass units (amu), making carbon-12 the standard (or reference) for the amu scale. On this scale, a helium-4 atom has a mass of 4.00 amu (1/3 of 12). Other measurements have shown that oxygen-16 atoms are 1.33 times heavier than carbon-12 atoms, making the mass of an oxygen-16 atom 16,00 amu. In this way, the masses of atoms of all the elements have been established.

Average Atomic Mass. The atomic masses that appear in the modern periodic table reflect the fact that elements occur in nature as combinations of isotopes. The atomic mass reported in the table is a weighted average of the atomic masses of the isotopes that make up the element. The mass of each isotope is weighted (or scaled) by its percent abundance in nature.

For example, the element lithium has two isotopes that occur in nature: ${}_{3}^{6}$ Li with 7.5 percent abundance, and ${}_{3}^{7}$ Li with 92.5 percent abundance. The atomic mass of lithium-6 is 6.01513 amu, and that of lithium-7 is 7.01601 amu. The average mass of such a mixture of Li atoms is given by:

average atomic mass = (fraction of isotope X)(mass of isotope X) + (fraction of isotope Y)(mass of isotope Y)

> = (0.075)(6.01513 amu) + (0.925)(7.0161 amu) = 0.45 amu + 6.49 amu = 6.94 amu

Note that neither ${}_{3}^{6}Li$ nor ${}_{3}^{7}Li$ has an atomic mass of 6.94 amu. This value is the weighted average of the masses of the two Li isotopes.

Molecular Masses. Molecules are composed of a number of atoms bonded together in a fixed arrangement. By the law of conservation of mass, the molecular mass is the sum of the atomic masses of the atoms in the molecular formula. For example, the molecular masses of two nitrogen oxides NO_2 and N_2O_5 are as follows:

Example

Exercises

3-1, 3-2

3.1

molecular mass of NO_2 = atomic mass of N + 2(atomic mass of O) = 14.01 amu + 2(16.00 amu) = 46.01 amu atomic mass of $N_2O_5 = 2($ atomic mass of N) + 5(atomic mass of O)= 2(14.01 amu) + 5(16.00 amu)

Example 3.2 Exercise 3-3

Avogadro's Number, the Mole and Molar Mass (Section 3.2)

= 108.02 amu

The Mole. The atomic mass scale is useful for small numbers of atoms or molecules, but is much too small for the quantities encountered in the laboratory, pharmacy or manufacturing plant. Macroscopic amounts of elements and compounds are too large to be measured conveniently on the atomic mass scale. For example, a vitamin C tablet would have a mass over 10²¹ amu. Macroscopic amounts of elements and compounds are measured in grams. but to measure out equal numbers of atoms of two elements, say carbon and oxygen, we cannot simply weigh out equal masses of the two elements. (Remember that oxygen atoms are 1.33 times heavier than carbon atoms.) Instead, we must measure a gram ratio of the two that is the same as the mass ratio of one C atom to one O atom. The atomic masses of C and O are 12.01 amu and 16.00 emu, respectively, so any amounts of C and O that have a mass ratio of 1.0; 1.33, will contain equal numbers of C and O atoms. Therefore, 16,00 g O contains the same number of atoms as 12.01 g C. The number of C atoms in 12.01 g C is 6.022×10^{23} , called Avogadro's number. The quantity of a substance that contains Avogadro's number of atoms or other entities is called a mole. The molar mass of an element or compound is the mass of one mole of its atoms or molecules. The molar mass of an element or molecule is also equal to its atomic or molecular mass expressed in grams rather than atomic mass units.

The following are examples of a mole of an element:

One mole of carbon contains 6.022×10^{23} atoms and has a mass of 12.01 $\rm g$ One mole of oxygen contains 6.022×10^{23} atoms and has a mass of 16.00 g

The term mole can be used in relation to any kind of particle, such as atoms, ions, or molecules. For clarity, the particle must always be specified. We say 1 mole of O_3 (ozone), or 1 mole of O_2 (diatomic oxygen), or 1 mole of Na⁺ (sodium ions). Other examples of molar amounts are:

 $\begin{array}{l} 1 \text{ mole Na}^{+} \text{ ions } = 6.022 \times 10^{23} \text{ Na}^{+} \text{ ions } = 23.00 \text{ g Na}^{+} \\ 1 \text{ mole } O_2 \text{ molecules } = 6.022 \times 10^{23} \text{ O}_2 \text{ molecules } = 32.00 \text{ g O}_2 \\ 0.5 \text{ mole } O_3 \text{ molecules } = 3.011 \times 10^{23} \text{ O}_3 \text{ molecules } = 24.00 \text{ g O}_3 \end{array}$

The mole is an SI unit that is defined in relation to the mass of the carbon-12 isotope. One mole is the amount of substance that contains as many elementary entities as there are atoms in 0.012 kg of carbon-12. In 0.012 kg of carbon-12 there are 6.022×10^{23} carbon-12 atoms. The symbol for mole is mol.

Examples 3.3 ~ 3.6 Exercises 3-4 - 3-9

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The Mass Spectrometer (Section 3.4)

The mass spectrometer is an electronic instrument for measuring the mass of ionized, gas phase compounds. It is the most accurate method available for determining atomic and molecular masses. There are many different types of mass spectrometers. All mass spectrometers consist of the same basic 4 parts: an ionization chamber to convert neutral samples to ions; ion optics to direct the ions into the mass analyzer; a mass analyzer to sort the ions by mass-to-charge ratio and a detector to count the different types of ions sorted by the analyzer. The type of ionizer and mass analyzer determine the type of sample the mass spectrometer is best suited to analyze.



The instrument depicted in Figure 3.3 of the text is called a magnetic sector spectrometer because ions of different mass-to-charge ratios (m/Z) are deflected into different paths by the magnet. This occurs because magnetic fields change the motion of charged particles. The arrival of ions at the detector produces an electrical signal (current) that is proportional to the number of ions, so we can determine the abundance of each type of ion in the sample as well as the mass.

Percent Composition & Chemical Formulas (Sections 3.5 – 3.6)

Percent Composition. The percent composition of a compound is the percentage by mass of each element in the compound. It measures the relative mass of an element in a compound. The formula for the percent composition of an element is:

% composition of element = $\frac{n \times element \ molar \ mass}{compound \ molar \ mass} \times 100\%$

Consider sodium chloride (NaCl) as an example. The molar mass, 58.44 g, is the sum of the mass of 1 mole of Na, 22.99 g, and the mass of 1 mole of Cl, 35.45 g. The percentage of Na by mass is

$$\% \text{Na} = \frac{1 \times 22.99 \text{ gNa}}{58.44 \text{ gNaCl}} \times 100\% = 39.33\%$$

The percentage of CI by mass is

$$\%CI = \frac{1 \times 35.45 \text{ gCI}}{58.44 \text{ gNaCI}} \times 100\% = 60.66\%$$

The percentages sum to 99.99% rather than 100% because the atomic masses and molar mass of NaCl were rounded to two decimal places.

Percent Composition & Chemical Formulas. Percent composition can be calculated directly from the formula of the compound (as above) or can be determined by chemical analysis if the formula is not known. You might expect, then, that given the percent

Examples 3.7, 3.8

Exercise 3-10 composition you could calculate the molecular formula. This is almost true. Remember, the percent composition is a measure of the relative contribution of an element to a compound. So we can calculate the empirical formula, reflecting the simplest whole-number ratio of the different kinds of atoms in the compound, from the percent composition. For example, nitrogen oxide has a percent composition of 30.43% N and 60.56% O. Since we know the molar masses of N and O, we can determine the relative numbers of N and O in a typical amount of this compound. The numbers of moles of N and O in 100.00 g of this compound are

#moles N = $\frac{0.3043 \times 100.00 \text{ gN}_{\text{X}}\text{O}_{\text{y}}}{14.01 \text{ gN/mol N}}$ = 2.17 mol N \Rightarrow 1 mol N #moles O = $\frac{0.6956 \times 100.00 \text{ gN}_{\text{X}}\text{O}_{\text{y}}}{16.00 \text{ gO/mol O}}$ = 4.35 mol O \Rightarrow 2 mol O

Dividing the number of moles of O by the number of moles of N shows that there are two oxygen atoms for every nitrogen atom in this compound, so the empirical formula is NO₂.

When the molar mass and the percent composition are known, the molecular formula can be calculated. Going back to the nitrogen oxide compound, the molar mass was determined to be 92.00 by mass spectrometry.

 $\# \text{moles} N_X O_y = \frac{100.00 \text{ gN}_X O_y}{92.00 \text{ gN}_X O_y/\text{mol} N_X O_y} = 1.08 \text{mol} N_X O_y \Rightarrow 1 \text{mol} N_X O_y$ $\# \text{moles} N = \frac{0.3043 \times 100.00 \text{ gN}_X O_y}{14.01 \text{ gN/mol} N} = 2.17 \text{mol} N \Rightarrow 2 \text{mol} N$ $\# \text{moles} O = \frac{0.6956 \times 100.00 \text{ gN}_X O_y}{16.00 \text{ gO/mol} O} = 4.35 \text{mol} O \Rightarrow 4 \text{mol} O$

Dividing the number of moles of O and N by the number of moles of oxide shows that there are two nitrogen atoms and four oxygen atoms for every molecule of this compound, so the molecular formula is N_2O_4 .

3.9 – 3.11 Exercises 3-11 – 3-15

Examples

Chemical Reactions and Chemical Equations (Section 3.7)

Chemical Equations. A chemical reaction is a process in which one, or more, chemical substance is changed into one, or more, new substance. A chemical equation is a symbolic shorthand for representing a chemical reaction. The chemical formulas of the reactants (starting materials) are written on the left side of the equation, and the formulas of the products on the right side. Equations are written according to the following format:

- Reactants and products are separated by an arrow. The arrow is read as "produces" or "yields."
- 2. Plus signs are placed between reactants and between products. A plus sign between reactants means that all the reactants are required for reaction. A plus between products implies that a mixture of two or more products is formed by the reaction. The plus sign is read as "plus" or "and."
- 3. Abbreviations are included to indicate the physical states of the reactants and products. These symbols, given in Table 3.1, are written in parentheses after the elements or compounds to which they refer.

Examples

Exercises

3.16 - 3.18

3.12 - 3.15

- 4. Balanced equations reflect the law of conservation of mass. That is, the number of atoms of a certain element appearing in the reactants must be equal to the number of atoms of that element appearing in the products.
- 5. Differences in the relative amounts of reactants consumed or products generated are reflected by stoichiometric coefficients. A coefficient is a number placed before a chemical formula in an equation that is a multiplier for the formula. For example, 3H₂O means three molecules of water, a total of 6 hydrogen atoms and three oxygen atoms. Subscripts, 2 in H₂O, represent the number of atoms in a compound. Absence of a coefficient or element subscript is understood to mean one.

Balancing Equations. When the hydrocarbon pentane (C_5H_{12}) is burned or combusted (reacted with O_2), carbon dioxide and water are produced. The unbalanced chemical equation representing the reaction is:

$$\cdot C_5 H_{12} + O_2 \rightarrow CO_2 + H_2O$$

Eventually, you will not need a procedure to balance chemical reactions. The basic idea is to change the coefficients of the reactants and products until the numbers of each type of atom are the same on each side of the reaction. It is important that you <u>NEVER</u> change the subscripts of the reactants or products; changing the subscripts changes the chemical compound. For now, use the following rules to balance equations, or develop your own. For simplicity, the physical state subscripts are omitted during this process.

- 1. Count and list the number of each type of atom on each side of the arrow.
- Look for elements that occur once on both sides of the equation; change the coefficients so that these elements are balanced, if necessary.
- 3. Change the coefficient of any remaining components to accommodate the changes made in step 2.
- Check the balanced equation to be sure the numbers of each atom are equal on both sides of the equation.

Step #	Equation	# rea	actant a	toms	# pr	oduct a	toms	Balanced?
1	$C_5H_{12} + O_2 \rightarrow CO_2 + H_2O$	5 C	12 H	20	1 C	2 H	30	No
2	$C_5H_{12} + O_2 \rightarrow 5CO_2 + H_2O$	5 C	12 H	20	5 C	2 H	11 0	No
3	$C_5H_{12} + O_2 \rightarrow 5CO_2 + 6H_2O$	5 C	12 H	20	5 C	12 H	16 O	No
4	$C_5H_{12} + 8O_2 \rightarrow 5CO_2 + 6H_2O$	5 C	12 H	16 O	5 C	12 H	16 O	Yes

Consider the combustion (burning) of pentane, a petroleum product:

Amounts of Reactants and Products (Section 3.8)

Mass Relationships in Reactions. Chemical equations contain information about the relative numbers of reactants and products involved in the reaction. The molar masses of the reactants and products link the numbers of reactants and products to their masses. Therefore, the balanced equation can be used to determine how many grams of one substance will be needed to react with a given mass of another, or how many grams of

product can be produced by the reaction of a specific mass of a reactant. For instance, the balanced equation

2 Al +	$Fe_2O_3 \rightarrow$	Al ₂ O ₃ +	2 Fe
2 mol	1 mol	1 mol	2 mol
53.96 g	159.70 g	101.96 g	111.70 g

states that 2 moles of Al, 53.96 g, will react completely with 1 mole of Fe_2O_3 , 159.70 g, and will yield 1 mole, 101.96 g, of Al₂O₃ and 2 moles, 111.70 g, of Fe.

The quantitative relationship between elements and compounds in chemical reactions is a part of chemistry called stoichiometry. The word stoichiometry derives from two Greek words: *stoicheion* (meaning "element") and *metron* (meaning "measure"). J. B. Richter (1762–1807) was the first to lay down the principles of stoichiometry. He said "stoichiometry is the science of measuring the quantitative proportions or mass ratios in which chemical elements stand to one another." In all stoichiometry problems, the balanced chemical equation provides the "bridge" that relates the amount of one reactant to the amount of another, and the amounts of products to reactants.

Mole Ratios. The balanced equation describing the reaction of aluminum and iron oxide defines the quantitative relationships between the reactants and products. We can see, for example, that 2 moles of AI are transformed to 1 mole of Al₂O₃. We can write these relationships in shorthand using mole ratios. Mole ratios are conversion factors that relate the number of reactants consumed to each other or to the number of product molecules formed.

$2AI + Fe_2O_3 \rightarrow Al_2O_3 + 2Fe$				
2 mol Al = $= 1 \mod Al_2O_3$	$\frac{2 \text{ mol Al}}{1 \text{ mol Al}_2 \text{O}_3}$	or	$\frac{1 \operatorname{mol} Al_2O_3}{2 \operatorname{mol} Al}$	
2 mol AI =;;= 2 mol Fe	2 mol Al 2 mol Fe	or	2 mol Fe 2 mol Al	
2 mol AI =::= 1 mol Fe ₂ O ₃	$\frac{2 \text{ mol Al}}{1 \text{ mol Fe}_2 \text{O}_3}$	or	$\frac{1 \text{ mol Fe}_2 \text{O}_3}{2 \text{ mol Al}}$	
1 mol Al ₂ O ₃ =::= 2 mol Fe	$\frac{1 \operatorname{mol} \operatorname{Al}_2 \operatorname{O}_3}{2 \operatorname{mol} \operatorname{Fe}}$	or	$\frac{2 \text{ mol Fe}}{1 \text{ mol Al}_2 \text{O}_3}$	

* the symbol =:= means "stoichiometrically equivalent to"

Mole ratios are used to answer stoichiometry questions such as

How many grams of iron are produced when 25.0 g Fe_2O_3 reacts with aluminum? How many grams of Al are required to react completely with 20.0 g Fe_2O_3 ?

Stoichiometry problems are solved in three steps:

- 1. Convert the amounts of given substances into moles, if necessary.
- 2. Use the appropriate mole ratio constructed from the balanced equation to calculate the number of moles of the needed or unknown substance.

3. Convert the number of moles of the needed substance into mass units if required.

How many grams of iron are produced when 25.0 g Fe₂O₃ reacts with aluminum?

1.
$$n_{Fe_2O_3} = 25.0 \text{ g Fe}_2O_3 \times \frac{1 \text{ mol Fe}_2O_3}{159.70 \text{ g Fe}_2O_3} = 0.157 \text{ mol Fe}_2O_3$$

2.
$$n_{Fe} = 0.157 \text{ mol Fe}_2O_3 \times \frac{2 \text{ mol Fe}}{1 \text{ mol Fe}_2O_3} = 0.314 \text{ mol Fe}$$

3.
$$m_{Fe} = 0.314 \text{ mol Fe} \times \frac{55.85 \text{ g Fe}}{1 \text{ mol Fe}} = 17.5 \text{ g Fe}$$

With practice, it will be easier to combine these three steps into a single calculation:

$$m_{Fe} = 25.0 \text{ gFe}_2O_3 \times \frac{1 \text{ mol Fe}_2O_3}{159.70 \text{ gFe}_2O_3} \times \frac{2 \text{ mol Fe}}{1 \text{ mol Fe}_2O_3} \times \frac{55.85 \text{ gFe}}{1 \text{ mol Fe}} = 17.5 \text{ gFe}$$

How many grams of AI are required to react completely with 20.0 g Fe₂O₃?

$$m_{AI} = 25.0 \text{ g Fe}_2 \text{O}_3 \times \frac{1 \text{ mol Fe}_2 \text{O}_3}{159.70 \text{ g Fe}_2 \text{O}_3} \times \frac{2 \text{ mol AI}}{1 \text{ mol Fe}_2 \text{O}_3} \times \frac{26.98 \text{ g AI}}{1 \text{ mol AI}} = 8.45 \text{ g AI}$$

Example 3.16 Exercises 3-19 – 3-22

Limiting Reagents & Reaction Yield (Sections 3.9 – 3.10)

Limiting Reagents. Usually the reactants are not present in the exact ratio prescribed by the balanced chemical equation. For example, a large excess of a less expensive reagent is used to ensure complete reaction of the more expensive reagent. In this situation, one reactant will be completely consumed before the other runs out. When this occurs, the reaction will stop and no more product will be made. The reactant that is consumed first is called the limiting reagent because it limits, or determines, the amount of product formed. The reactant that is not completely consumed is called the excess reagent. The figure below illustrates the relationships between reagents and products in this case.



Reconsidering the aluminum/iron oxide reaction, suppose that 1.2 moles of Al are reacted with 1 mole of Fe_2O_3 . In any stoichiometry problem, it is important to determine which reactant is the limiting one, to correctly predict the yield of products.

Step #	Equation	# reactant amounts		# product amounts	
model	$2 \text{ Al} + \text{Fe}_2\text{O}_3 \rightarrow \text{Al}_2\text{O}_3 + 2 \text{ Fe}$	2 mol Al	1 mol Fe ₂ O ₃	1 mol Al ₂ O ₃	2 mol Fe
start	$2 \text{ Al} + \text{Fe}_2\text{O}_3 \rightarrow \text{Al}_2\text{O}_3 + 2 \text{ Fe}$	1.2 mol Al	1 mol Fe ₂ O ₃	0 mol Al ₂ O ₃	0 mol Fe
reaction	$2 \text{ Al} + \text{Fe}_2\text{O}_3 \rightarrow \text{Al}_2\text{O}_3 + 2 \text{ Fe}$	1.2 mol Al	0.6 mol Fe ₂ O ₃	0 mol Al ₂ O ₃	0 mol Fe
finish	$2 \text{ AI} + \text{Fe}_2\text{O}_3 \rightarrow \text{AI}_2\text{O}_3 + 2 \text{ Fe}$	0 mol Al	0.4 mol Fe ₂ O ₃	0.6 mol Al ₂ O ₃	1.2 mol Fe

In this situation, there is more Fe_2O_3 than the aluminum can consume, so aluminum is depleted first. Therefore, aluminum is the *limiting reagent*. There is more Fe_2O_3 than needed to react completely with the given amount of Al, making Fe_2O_3 the excess reagent. Note that the limiting reactant (1.2 mol Al) is not the reactant in lesser molar amount (1.0 mol Fe_2O_3).

Percent Yield. The product amounts predicted from the balanced reaction are best case scenarios, the perfect world result. In practice, the actual yield is usually less than the calculated, or "theoretical" yield. The theoretical yield is calculated based on the assumption that all the limiting reagent reacts according to the balanced equation. The theoretical yield for the aluminum/iron oxide reaction above is 0.6 mol Al₂O₃ or 61.18 g of Al₂O₃. The percent yield is based on the actual amount of product produced in the reaction. The percent yield is defined as

% percent yield = $\frac{\text{actual yield}}{\text{theoretical yield}} \times 100\%$

So if the aluminum/iron oxide reaction above actually produced 52.5 g of Al_2O_3 , the percent yield is

% percent yield = $\frac{52.5 \text{ g}}{61.18 \text{ g}} \times 100\% = 85.8\%$

Example 3.18 Exercise

3-25

Example 3.17 Exercises

3-23 - 3-24

JI. JUIN ANNIN ON ALCINGO, MALL

to stress the wording "on average"?

WORKED EXAMPLES

EXAMPLE 3.1 Average Atomic Mass

The element boron (B) consists of two stable isotopes with atomic masses of 10.012938 amu and 11.009304 amu. The average atomic mass of B is 10.81 amu. Which isotope is more abundant, boron-10 or boron-11?

Solution

The atomic mass is an average of the masses of the naturally occurring isotopes of an element. Each isotopic mass is multiplied by its relative abundance. If both isotopes in this example had a natural abundance of 50 percent, then the atomic mass would be the average of the two masses, 10.5 amu. Since the atomic mass of boron (10.81 amu) is greater than 10.5, the abundance of the boron-11 isotope must be larger than that of the boron-10. The abundances of boron-10 and boron-11 are 19.6% and 80.4%, respectively.

EXAMPLE 3.2 Molecular Mass

Calculate the molecular mass of carbon tetrachloride (CCl₄).

Solution

The molecular mass is the sum of the atomic masses of all the atoms in the molecule: molecular mass $CCl_4 = (atomic mass of C) + 4(atomic mass of Cl)$ = (12.01 amu) + 4(35.45 amu)

molecular mass $CCl_4 = 153.81$ amu

EXAMPLE 3.3 The Molar Mass

Naturally occurring lithium consists of 7.5 percent Li-6 atoms, and 92.5 percent Li-7 atoms. Complete the following sentences:

- a. The number of Li atoms in one mole of Li is
- b. One mole of Li atoms consists of _____ Li-6 atoms and _____ Li-7 atoms and will have a mass of _____ g.

Solution

a. One mole of Li contains 6.022 × 10²³ Li atoms (a mixture of Li-6 atoms and Li-7 atoms).



b. One mole of Li atoms contains $(0.074)(6.022 \times 10^{23})$ Li-6 atoms, which is equal to 4.5×10^{22} Li-6 atoms; and $(0.925)(6.022 \times 10^{23})$ Li-7 atoms, which is 5.57×10^{23} Li-7 atoms. Note that the total number of Li atoms is 6.022×10^{23} , and thus will have a mass of <u>6.94</u> g.

EXAMPLE 3.4 Mass of a Given Number of Moles

What is the mass of 2.25 moles of iron (Fe)?

Solution

To convert moles of Fe to grams of Fe, first write the relationship between moles, atoms, and mass.

1 mol Fe = 6.022×10^{23} Fe atoms = 55.85 g Fe

The problem asks:

? g Fe = 2.25 mol Fe

Since the atomic mass of iron is 55.85 amu, then 1 mol of iron has a mass of 55.85 g. The unit conversion factor is

 $\frac{55.85 \text{ g}}{1 \text{ mol Fe}} = 1$

Since 1 mol Fe has a mass of 55.85 g, then 2.25 mol Fe must have a mass of:

? g Fe = 2.25 mol Fe $\times \frac{55.85 \text{ g}}{1 \text{ mol Fe}}$ = 126 g Fe

EXAMPLE 3.5 Number of Atoms in a Given Mass

How many zinc atoms are present in 20.0 g Zn?

Solution

We know that 1 mole of Zn contains 6.022×10^{23} atoms. First, find the number moles of Zn atoms in 20.0 g Zn, and then multiply by Avogadro's number. Finding the number of moles of zinc is the key to finding the number of atoms. The relationship between moles, atoms, and grams is:

1 mol Zn = 6.022×10^{23} Zn atoms = 65.39 g Zn

The problem asks:

? Zn atoms = 20.0 g Zn The solution strategy (roadmap) is:

g Zn \rightarrow mol Zn \rightarrow number of Zn atoms

One mol of Zn has a mass of 65.39 g. Therefore, 20.0 g Zn corresponds to:

? Zn mol = 20.0 g Zn
$$\times \frac{1 \text{ mol } \text{Zn}}{65.39 \text{ g Zn}} = 0.3059 \text{ mol } \text{Zn}$$

Here we will carry one more digit than the correct number of significant figures. To convert moles of zinc to atoms of zinc, we use Avogadro's number, the number of atoms per mole, as the unit factor:

 $\frac{6.022 \times 10^{23} \text{ Zn atoms}}{1 \text{ mol Zn}} = 1$

? Zn atoms = 0.3059 mol Zn × $\frac{6.022 \times 10^{23} \text{ Zn atoms}}{1 \text{ mol Zn}}$ = 1.84 × 10²³ Zn atoms

•Comment

Instead of calculating the number of moles separately, we could have strung the conversion factors together into one calculation:

$$? \text{ Zn atoms} = 20.0 \text{ g Zn} \times \frac{1 \text{ mol Zn}}{65.39 \text{ g Zn}} \times \frac{6.022 \times 10^{23} \text{ Zn atoms}}{1 \text{ mol Zn}}$$

 $= 1.84 \times 10^{23}$ Zn atoms

EXAMPLE 3.6 Moles of a Molecular Compound

a. How many molecules of ethane (C₂H₆) are present in 50.3 g of ethane?

b. How many atoms each of H and C are in this sample?

Solution (a)

The problem asks:

? C_2H_6 molecules = 50.3 g C_2H_6

To convert grams to molecules, you need the molar mass.

The molecular mass of C₂H₆ is:

2(12.01 amu) + 6(1.008 amu) = 30.07 amu

Therefore, we can write:

1 mol C₂H₆ = 6.022×10^{23} C₂H₆ molecules = 30.07 g C₂H₆

Finding the number of moles of C_2H_6 is the key to finding the number of molecules.

 $g C_2H_6 \rightarrow mol C_2H_6 \rightarrow number of C_2H_6$ molecules

? mol $C_2H_6 = 50.3 \text{ g} C_2H_6$

Since 1 mol C_2H_6 is 30.07 g, then 50.3 g C_2H_6 must be:

? mol C₂H₆ = 50.3 g C₂H₆ ×
$$\frac{1 \text{ mol } C_2H_6}{30.07 \text{ g } C_2H_6}$$
 = 1.67 mol C₂H₆

Since 1 mol C₂H₆ contains 6.022×10^{23} molecules, then 1.67 mol must contain:

? C₂H₆ molecules = 1.67 mol C₂H₆ ×
$$\frac{6.022 \times 10^{23} \text{ molecules}}{1 \text{ mol C}_2\text{H}_6}$$

=
$$1.01 \times 10^{24} \text{ C}_2\text{H}_6$$
 molecules

Solution (b)

ų,

The molecular formula shows the number and kinds of atoms in a molecule.

 $\frac{6 \text{ H atoms}}{\text{C}_2\text{H}_6 \text{ molecule}} \text{ and } \frac{2 \text{ C atoms}}{\text{C}_2\text{H}_6 \text{ molecule}}$

Multiplying the number of C_2H_6 molecules by the number of atoms of each kind per molecule gives the number of each kind of atom present.

 1.01×10^{24} molecules $\times \frac{6 \text{ H atoms}}{\text{C}_2\text{H}_6 \text{ molecule}} = 6.06 \times 10^{24} \text{ H atoms}$

 1.01×10^{24} molecules $\times \frac{2 \text{ C atoms}}{C_2 H_6}$ = 2.02×10^{24} C atoms

EXAMPLE 3.7 Percent Composition

Calculate the percent composition of glucose (C₆H₁₂O₆).

Solution

First the molar mass of glucose must be found from the atomic masses of each element.

molar mass of C₆H₁₂O₆ = $\begin{bmatrix} 6 \mod C \times \frac{12.01 \text{ g}}{1 \mod C} \end{bmatrix} + \begin{bmatrix} 12 \mod H \times \frac{1.008 \text{ g}}{1 \mod H} \end{bmatrix} + \begin{bmatrix} 6 \mod O \times \frac{16.00 \text{ g}}{1 \mod O} \end{bmatrix}$ = 72.06 g + 12.10 g + 96.00 g = 180.16 g Then the percent of each element present is found by dividing the mass of each element in 1 mole of glucose by the total mass of 1 mole of glucose.

mass percent of C = $\frac{\text{mass of C in 1 mol } C_6H_{12}O_6}{\text{mass of 1 mole } C_6H_{12}O_6} \times 100\%$

$$%C = \frac{6 \text{ mol } C \times (12.01 \text{ g/mol } C)}{180.16 \text{ g } C_6 \text{H}_{12} \text{O}_6} \times 100\% = \frac{72.06 \text{ g}}{180.16 \text{ g}} \times 100\% = 40.00\% \text{ C}$$

After practicing the calculation several times, you can simplify the notation:

$$\%$$
H = $\frac{12 \times 1.008 \text{ g}}{180.16 \text{ g}} \times 100\% = \frac{12.10 \text{ g}}{180.16 \text{ g}} \times 100\% = 6.72\%$ H

$$\%O = \frac{6 \times 16.00 \text{ g}}{180.16 \text{ g}} \times 100\% = \frac{96.00 \text{ g}}{180.16 \text{ g}} \times 100\% = 53.3\% \text{ O}$$

Thus glucose (C₆H₁₂O₆) contains 40.0% C, 6.72% H, and 53.3% O by mass.

Comment

A good way to check the results is to sum the percentages of the elements, because their total must add to 100%. Here we get 100.02%.

EXAMPLE 3.8 Using Percent Composition

Calculate the mass of carbon in 10.00 g of glucose ($C_6H_{12}O_6$).

Solution

In Example 3.7 we calculated that glucose contains 40.00% carbon. Therefore:

mass C = 40.00% of 10.00 g C₆H₁₂O₆ =
$$\frac{40.00 \text{ g C}}{100 \text{ g C}_6\text{H}_{12}\text{O}_6} \times 10.00 \text{ g C}_6\text{H}_{12}\text{O}_6 = 4.000 \text{ g C}$$

This calculation would have to be done from scratch if we did not already know the percentage of carbon. The road map is:

mass of glucose \rightarrow mol glucose \rightarrow mol carbon \rightarrow g carbon

? mass C = 10.00 g C₆H₁₂O₆ ×
$$\frac{1 \text{ mol } C_6H_{12}O_6}{180.16 \text{ g } C_6H_{12}O_6} \times \frac{6 \text{ mol } C}{1 \text{ mol } C_6H_{12}O_6} \times \frac{12.01 \text{ g } C}{1 \text{ mol } C} = 4.000 \text{ g } C$$

EXAMPLE 3.9 Empirical Formula

An elemental analysis of a new compound reveals its percent composition to be: 50.7% C, 4.23% H, and 45.1% O. Determine the empirical formula.

Solution

The empirical formula gives the relative numbers of atoms of each element in a formula unit. To start, assume you have exactly 100 g of compound, and then determine the number of moles of each element present. Then find the ratios of the number of moles.

50.7 g C ×
$$\frac{1 \text{ mol C}}{12.01 \text{ g C}}$$
 = 4.22 mol C

$$4.23 \text{ g H} \times \frac{1 \text{ mol H}}{1.008 \text{ g H}} = 4.20 \text{ mol H}$$

$$45.1 \text{ g O} \times \frac{1 \text{ mol O}}{16.00 \text{ g O}} = 2.82 \text{ mol O}$$

This gives the mole ratio for C : H : O of 4.22 : 4.20 : 2.82. Dividing by the smallest of the molar amounts gives:

 $\frac{4.22 \text{ mol C}}{2.82 \text{ mol O}} = 1.50 \text{ mol C to } 1.00 \text{ mol O and } \frac{4.20 \text{ mol H}}{2.82 \text{ mol O}} = 1.49 \cong 1.5 \text{ mol H to } 1.00 \text{ mol O}$

Therefore, $C_{1.5}H_{1.5}O_{1.0}$ is a possible formula.

This is not an acceptable formula because it does not contain all whole numbers. To convert these fractions to whole numbers, multiply each subscript by the same number, in this case a 2. The empirical formula therefore is $C_3H_3O_2$.

EXAMPLE 3.10 Molecular Formula

Mass spectrometer experiments on the compound in Example 3.9 show its molecular mass to be about 140 amu. What is the molecular formula?

Solution

First find how many empirical formula units there are in 1 mole of compound which is 140 g. The molar mass of the empirical formula $C_3H_3O_2$ is 71 g.

Dividing 140 g by 71 g indicates there are two empirical units per molecule. Therefore, the molecular formula must have twice as many atoms as the empirical formula.

molecular formula = $C_6H_6O_4$

EXAMPLE 3.11 Carbon-Hydrogen Analysis

When a 0.761-g sample of a compound of carbon and hydrogen is burned in a C–H combustion apparatus (see Figure 3.5 in the text), 2.23 g CO₂ and 1.37 g H₂O are produced. Determine the percent composition of the compound.

Solution

Here we want the masses of carbon and hydrogen in the original compound. All the carbon is now present in 2.23 g of CO₂. All the hydrogen is now present in 1.37 g of H₂O. How many grams of C are there in 2.23 g of CO₂, and how many grams of H are there in 1.37 g of H₂O? We know there is 1 mole of C atoms (12.01 g) in every mole of CO₂, or 44.01 g.

The solution road map is:

$$g CO_2 \rightarrow mol CO_2 \rightarrow g C$$

? g C = 2.23 g CO₂ ×
$$\frac{1 \text{ mol CO}_2}{44.01 \text{ g CO}_2}$$
 × $\frac{12.01 \text{ g C}}{1 \text{ mol CO}_2}$ = 0.608 g C

? g H = 1.37 g H₂O ×
$$\frac{1 \text{ mol } \text{H}_2\text{O}}{18.0 \text{ g } \text{H}_2\text{O}}$$
 × $\frac{2.01 \text{ g H}}{1 \text{ mol } \text{H}_2\text{O}}$ = 0.153 g H

The percentage composition is:

$$\%H = \frac{0.153 \text{ g H}}{0.761 \text{ g compound}} \times 100\% = 20.1\% \text{ H}$$

%C =
$$\frac{0.608 \text{ g C}}{0.761 \text{ g compound}} \times 100\% = 79.9\% \text{ C}$$

EXAMPLE 3.12 Balancing Chemical Equations

Balance the following reaction. In this displacement reaction, zinc displaces H_2 from chemical combination with chlorine.

 $Zn(s) + HCl(aq) \rightarrow ZnCl_2(aq) + H_2(g)$

Solution

Step 1: Identify elements that occur in only two compounds in the equation. In this case, each of the three elements Zn, H, and Cl occurs in only two compounds. **Step 2:** Of these, balance the element with the largest subscript. Both Cl and H have the subscript 2, so balance either one of them first. Multiplying HCl by 2 to balance H:

$$Zn + 2 HCI \rightarrow ZnCl_2 + H_2$$

Taking stock:

Reactants	Products
H (2)	H (2)
CI (2)	CI (2)
Zn (1)	Zn (1)

At this point, both H and CI are balanced. Further inspection reveals that Zn is also balanced. Thus, the equation is balanced!

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EXAMPLE 3.13 Balancing Chemical Equations

The reaction of a hydrocarbon with oxygen is an example of a combustion reaction. Balance the equation for the reaction of pentane with oxygen gas:

$$C_5H_{12} + O_2 \rightarrow CO_2 + H_2O$$

Solution

Following step 1 given in the previous example, we note that both H and C appear in only two compounds. According to step 2, we note that of these, H has the largest subscript. Balance H first by placing the coefficient 6 in front of H₂O. Next balance the carbon atoms by placing a 5 in front of CO_2 .

 $C_5H_{12} + O_2 \rightarrow 5 CO_2 + 6 H_2O$

Taking stock:

<u>Reactants</u>	<u>Products</u>
C (5)	C (5)
H (12)	H (12)
O (2)	O (16)

Finally, the oxygen atoms can be balanced. The products already have their coefficients determined, and so the reactants must be adjusted to supply 16 O atoms. Eight molecules of O₂ contain 16 O atoms, and so write the coefficient 8 in front of O₂.

 $C_5H_{12} + 8 O_2 \rightarrow 5 CO_2 + 6 H_2O$

Reactants	Products
C (5)	C (5)
H (12)	H (12)
O (16)	O (16)

EXAMPLE 3.14 Balancing Chemical Equations

Balance the following decomposition reaction:

 $NaClO_3(s) \rightarrow NaCl(s) + O_2(g)$

Solution

According to steps 1 and 2, O should be balanced first. There are 3 O atoms on the reactant side and 2 on the product side. When an element that occurs in only two substances in the equation and the number of atoms of that element is even on one side and odd on the other side of the equation, use two coefficients that increase the number of atoms on each side of the equation to the least common multiple.

 $\begin{array}{ccc} \text{NaClO}_3 \rightarrow & \text{NaCl} + \text{O}_2 \\ \underline{\text{Reactants}} & \underline{\text{Products}} \\ \text{O} (3) & & \text{O} (2) \end{array}$

The least common multiple for balancing O is $3 \times 2 = 6$. The two coefficients are 2 and 3.

 $\begin{array}{rrr} 2 \text{ NaClO}_3 \rightarrow & \text{NaCl} + 3 \text{ O}_2 \\ \hline \underline{\text{Reactants}} & & \underline{\text{Products}} \\ O (6) & & O (6) \end{array}$

Balancing the Na and CI atoms gives:

 $2 \text{ NaClO}_3 \rightarrow 2 \text{ NaCl} + 3 \text{ O}_2$

EXAMPLE 3.15 Balancing Chemical Equations

Balance the following precipitation reaction in which sulfuric acid reacts with barium chloride in aqueous solution to yield hydrochloric acid and a precipitate of barium sulfate.

$$H_2SO_4(aq) + BaCl_2(aq) \rightarrow HCl(aq) + BaSO_4(s)$$

Solution

Here, it helps to recognize certain groups of atoms that maintain their identity during the reaction. In this equation the sulfate ion, SO_4^{2-} , appears as a unit.

 $H_2SO_4 + BaCl_2 \rightarrow HCl + BaSO_4$

Products
H (1)
SO ₄ ²⁻ (1)
Ba (1)
CI (Ì)

Either H or CI could be balanced first. Balance chlorine by multiplying HCI by 2:

 $H_2SO_4 + BaCl_2 \rightarrow BaSO_4 + 2 HCl$

A check of the H atoms shows they are now balanced along with the other elements.

EXAMPLE 3.16 The Mole Method

Sulfur dioxide can be removed from refinery stack gases by reaction with quicklime, CaO.

 $SO_2(g) + CaO(s) \rightarrow CaSO_3(s)$

If 975 g of SO₂ is to be removed from stack gases by the above reaction, what mass of CaO is required to completely react with it?

Solution

First be certain that the equation is correctly balanced. Then follow the three steps as outlined in the above section.

 SO_2 + CaO \rightarrow CaSO₃

step 1 step 2 step 3

$$g SO_2 \rightarrow mol SO_2 \rightarrow mol CaO \rightarrow g CaO$$

- 1. Convert the 975 g of SO₂ to moles using its molar mass-
- 2. Use the chemical equation to find the number of moles of CaO that reacts per mole of SO₂.
 - From the balanced equation we can write: 1 mol CaO = 1 mol SO2
- 3. Convert moles of CaO to grams of CaO using the molar mass of CaO.

Write out an equation which restates the problem:

? g CaO = 9.75×10^2 g SO₂

String the conversion factors from the three steps one after the other.

$$? g CaO = 9.75 \times 10^{2} g SO_{2} \times \frac{1 \text{ mol } SO_{2}}{64.07 g SO_{2}} \times \frac{1 \text{ mol } CaO}{1 \text{ mol } SO_{2}} \times \frac{56.08 \text{ g CaO}}{1 \text{ mol } CaO}$$

 $= 8.53 \times 10^2$ g CaO

EXAMPLE 3.17 Limiting Reagent

Phosphine (PH₃) burns in oxygen to produce phosphorus pentoxide (P_2O_5) and water.

$$2 PH_3(g) + 4 O_2(g) \rightarrow P_2O_5(s) + 3 H_2O(\ell)$$

How many grams of P_2O_5 will be produced when 17.0 g of phosphine is mixed with 16.0 g of O_2 and reaction occurs?

Solution

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When the amounts of both reactants are given, it is possible that one will be completely used up before the other. The limiting reagent will be completely consumed and will determine the amount of products. To find the limiting reagent, first find the number of moles of each reagent available.

17.0 g PH₃ ×
$$\frac{1 \text{ mol PH}_3}{33.99 \text{ g PH}_3}$$
 = 0.500 mol PH₃

16.0 g
$$O_2 \times \frac{1 \text{ mol } O_2}{32.00 \text{ g } O_2} = 0.500 \text{ mol } O_2$$

The balanced equation gives the stoichiometric ratio of moles of O₂ required to react per mole of PH₃.

stoichiometric ratio = $\frac{2 \mod O_2}{1 \mod PH_3}$

The amount of O₂ required for complete reaction of the given amount of PH₃ is:

$$0.500 \text{ mol PH}_3 \times \frac{2 \text{ mol O}_2}{1 \text{ mol PH}_3} = 1.00 \text{ mol O}_2$$

Since only 0.500 mol O_2 is given, then O_2 is the limiting reagent. When all of the O_2 is consumed, some PH₃ will be left unreacted (the excess reagent). The theoretical yield of P_2O_5 is calculated by assuming complete reaction of the limiting reagent. The road map is:

$$g O_2 \rightarrow mol O_2 \rightarrow mol P_2O_5 \rightarrow g P_2O_5$$

? g P₂O₅ = 0.500 mol O₂ ×
$$\frac{1 \text{ mol } P_2O_5}{4 \text{ mol } H_2}$$
 × $\frac{141.9 \text{ g } P_2O_5}{1 \text{ mol } P_2O_5}$

= 17.7 g P₂O₅

EXAMPLE 3.18 Percent Yield

In the reaction of 4.0 moles of N_2 with 6.0 moles of H_2 , a chemist obtained 1.6 moles of NH_3 . What is the percent yield of NH_3 ?

 $3 H_2 + N_2 \rightarrow 2 NH_3$

Solution

To calculate the percent yield, you must first calculate the theoretical yield. The theoretical yield of NH₃ is determined by the limiting reagent. From the balanced equation we see that the stoichiometric ratio is 3 mol H₂ to 1 mol N₂. The 4.0 mol N₂ given requires 12.0 mol H₂ for complete reaction. Since only 6.0 mol H₂ are given, then H₂ is the limiting reactant. In this case, 6.0 mol H₂ will react with 2.0 mol N₂ yielding 4.0 mol NH₃.

theoretical yield = 6.0 mol H₂ × $\frac{2 \text{ mol NH}_3}{3 \text{ mol H}_2}$ = 4.0 mol NH₃

The percent yield is found by dividing the actual yield by the theoretical yield and multiplying by 100 percent.

% yield NH₃ = $\frac{\text{actual yield NH}_3}{\text{theoretical yield NH}_3} \times 100\%$

$$= \frac{1.6 \text{ mol NH}_3}{4.0 \text{ mol NH}_3} \times 100\%$$

% yield $NH_3 = 40\%$