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Chapter 3

Mass Relations in Chemistry; Stoichiometry

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Outline



3.1 Atomic mass 原子量

1. Atomic Masses ; the Carbon-12 Scale
2. Atomic Masses and Isotopic Abundances
3. Masses of Individual Atoms ; Avogadro,s Number

3.2 The mole

1. Mole-Gram Conversions

3.3 Mass relations in chemical formula

1. Percent composition from Formula
2. Simplest Formula from Chemical Analysis
3. Molecular Formula form Simplest formula

3.4 Mass relations in reactions

- Writing and Balancing Chemical Equations
- Mass Relations form Equations
- Limiting Reactant and Theoretical Yield

Introduction



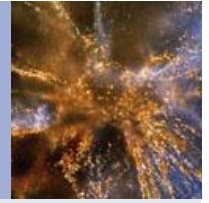
- **Chemistry is a quantitative science. Atoms of elements differ from one another not only in composition (number of protons ,electrons, neutrons) ,but also in mass, Chemical formulas of compounds tell us not only the atom ratios in which elements are present but also the mass ratios.**

Fundamental Questions



- How many atoms are there in a gram of an element?
- How much iron can be obtained from a ton of iron ore?
- How much nitrogen gas is required to form a kilogram of ammonia?
- **Stoichiometry**
- Chemical arithmetic
- Study of mass relationships in chemistry

3.1 Atomic Masses



- Individual atoms are too small to be weighed on a balance.
- Collections of atoms can be weighed and those collections can give accurate atomic masses

1. Carbon



- ^{12}C has a mass of exactly 12.000 amu
- Carbon in the periodic table has a mass of 12.011 amu
 - Why isn't it exactly 12.000?
 - Why are most atomic masses not whole numbers?

Average Atomic Masses

- The atomic mass quoted in the periodic table is the **weighted average of the atomic masses of all isotopes of that element**
- $\text{C} = (0.9890 \times 12.00) + (0.0110 \times 13.00335) = 12.011$

The Carbon-12 Scale



- **Relative masses** of atoms of different elements are expressed in terms of their atomic masses .
- The atomic mass of an element indicates how heavy, on average, an atom of an element is when compared to an atom of another element
- **Unit** is the amu (**a**tomic **m**ass **u**nit)
- Mass of one ^{12}C atom = 12 amu (exactly)
- Note that ^{12}C and C-12 mean the same thing

Masses and the Periodic Table



- The mass of an element is indicated below the symbol for the element
- Consider He
 - On average, one He atom weighs 4.003 amu
 - This is about 1/3 the mass of a carbon-12 atom

$$\frac{4.003 \text{ amu}}{12.00 \text{ amu}} = 0.3336$$

- Consider H
 - On average, one H (0.0840×12.0) atom weighs 1.008 amu

$$\frac{4.003 \text{ amu}}{1.008 \text{ amu}} = 3.971$$

Comparing Two Atoms – Mass Ratio



$$\frac{\text{atomic mass X}}{\text{atomic mass Y}} = \frac{\text{mass of atom X}}{\text{mass of atom Y}}$$

2. Atomic masses and Isotopic Abundances



- A mass spectrometer is used to determine atomic masses

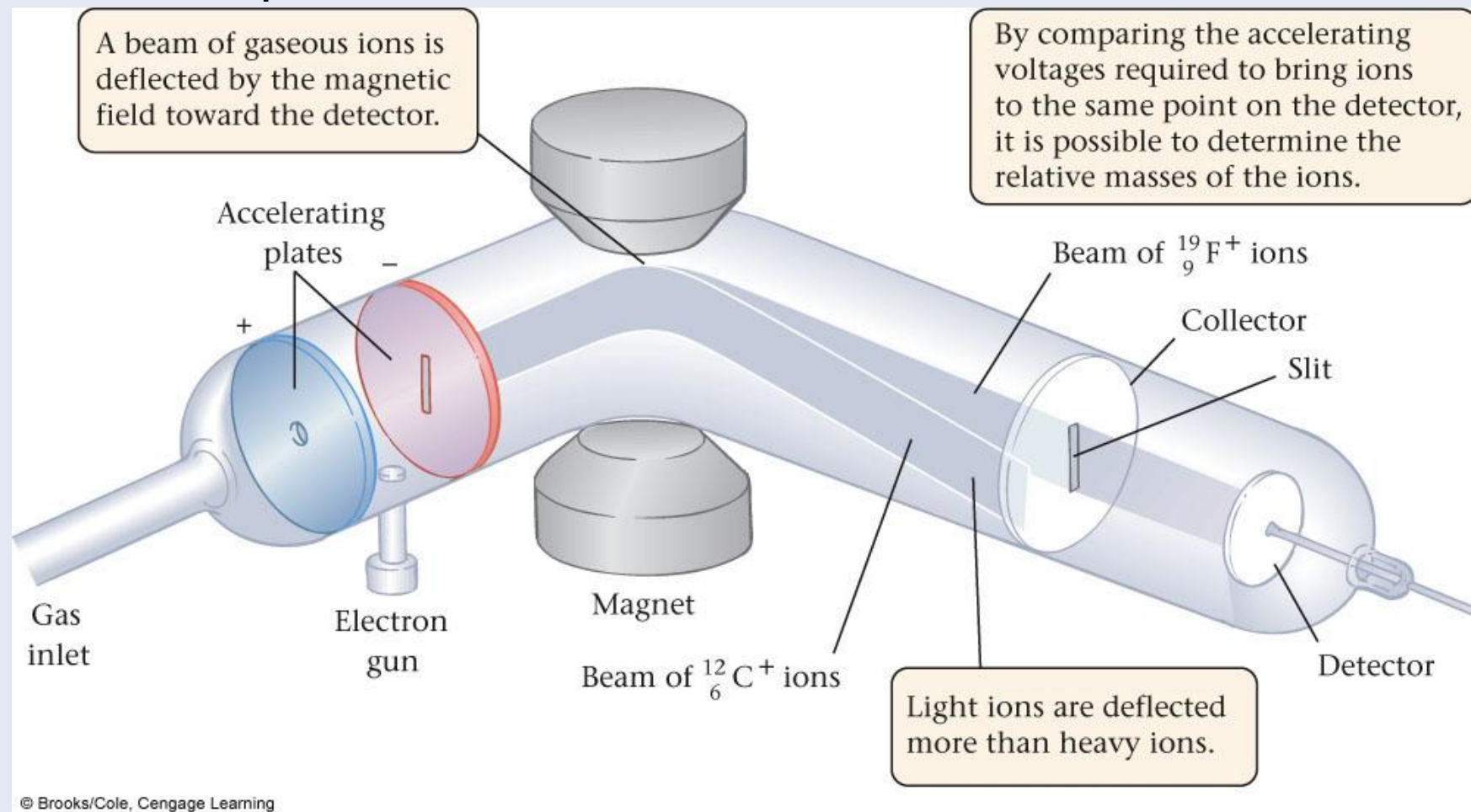


Figure 3.1 – Mass Spectrometer

Mass Spectrometry

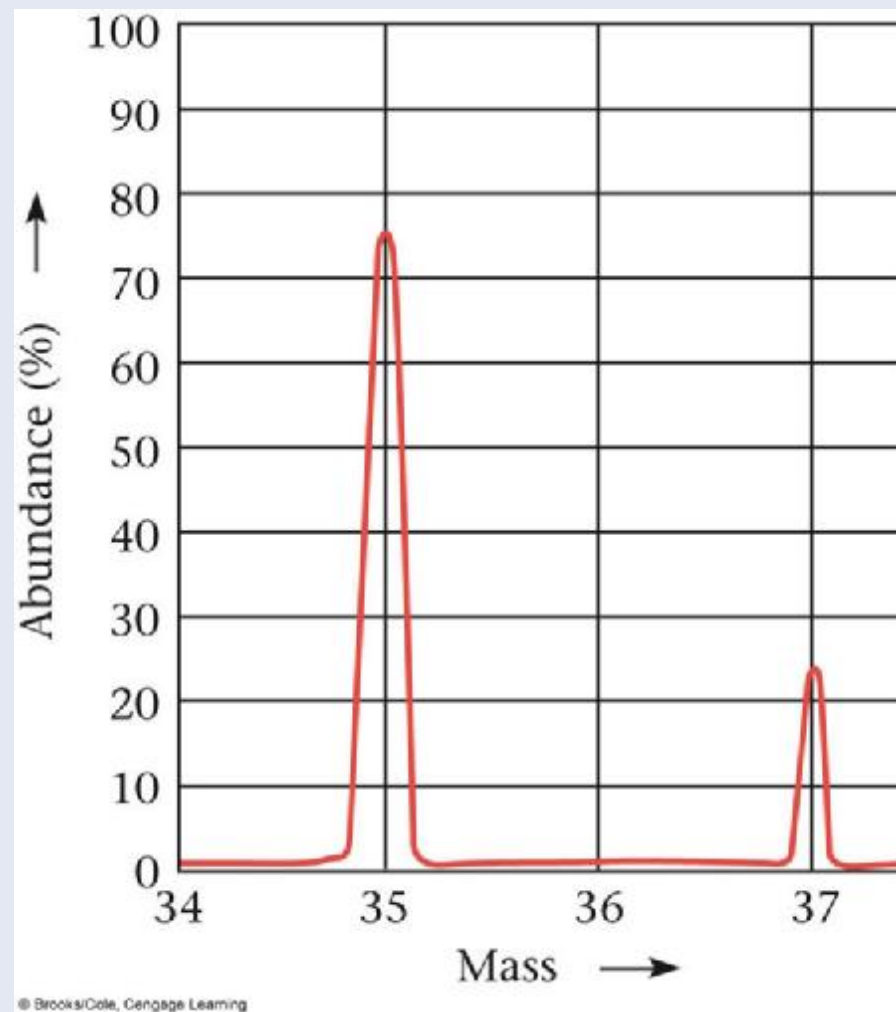


- Atoms are ionized at low pressure in the gas phase
- The cations that form are accelerated toward a magnetic field
- The extent to which the cation beam is deflected is inversely related to the mass of the cation

Figure 3.2 – Mass Spectrum of Cl



- The area under the peak in the mass spectrogram gives the isotopic abundance



Isotopes



- Recall that an isotope is an atom with the same number of protons
 - Therefore, the same element
- Different mass number
 - Therefore, a different number of neutrons

- Using MS Fluorine is 1.583 times C
- $1.583 \times 12.00 = 19.0 \text{ amu}$
- Atomic fluorine exists as a single isotope
- Mass of F is exactly 19.00 amu

Isotopic Abundance



- To determine the mass of an element, we must know the mass of each isotope and the atom percent of the isotopes (***isotopic abundance***)
- The mass spectrometer can determine the isotopic abundance
- Two isotopes
 - Cl-35 ,Cl-37

	Atomic Mass	Abundance
Cl-35	34.97 amu	75.53%
Cl-37	36.97 amu	24.47%

$$\begin{aligned} \text{atomic mass Cl} &= 34.97 \text{ amu} \left(\frac{75.53}{100} \right) + 36.97 \left(\frac{24.47}{100} \right) \text{ amu} \\ &= 35.46 \text{ amu} \end{aligned}$$

Weighted Averages



- For an element with two isotopes, Y_1 and Y_2 :

$$\text{atomic mass } Y = (\text{atomic mass } Y_1) \frac{\% Y_1}{100} + (\text{atomic mass } Y_2) \frac{\% Y_2}{100}$$

- For chlorine:

$$\begin{aligned} \text{atomic mass } Cl &= 34.97 \text{ amu} \left(\frac{75.53}{100} \right) + 36.97 \left(\frac{35.46}{100} \right) \text{ amu} \\ &= 35.46 \text{ amu} \end{aligned}$$

Example 3.1



- Bromine (Br, atomic mass = 79.90 amu) consists of two isotopes: Br-79 (78.92 amu) and Br-81 (80.92 amu). What is the abundance of the heavier isotope?
- Br-81 x % Br-79 佔 $(100-x)$ %

$$\begin{aligned} 79.90 \text{ amu} &= 78.92 \text{ amu} \times \frac{(100 - x)}{100} + 80.92 \times \frac{x}{100} \\ &= 78.92 \text{ amu} + 2.00 \text{ amu} \times \frac{x}{100} \end{aligned}$$

$$\frac{x}{100} = \frac{79.90 \text{ amu} - 78.92 \text{ amu}}{2.00 \text{ amu}} = 0.49$$

$$x = 49\%$$

3. Masses of Individual Atoms



- It is usually sufficient to know the relative masses of atoms and calculate the mass in grams of individual atoms.
 - One He atom is about four times as heavy as one H atom
 - Therefore
 - The mass of 100 He atoms is about four times the mass of 100 H atoms
 - The mass of a million He atoms is about four times the mass of a million H atoms

3. Masses of individual atoms; Avogadro's number



(1) A sample of any element with a mass in grams equal to its atomic mass contains the number of atoms.

no. of He atoms in 4.03g = no. of H atoms in 1.008g

Avogadro's number N_A , 6.022×10^{23} (four significant figures)

(2). It represents the number of atoms of an element in a sample whose mass in grams is numerically equal to the atomic mass of the element.

- 6.022×10^{23} H atoms in 1.008 g H
- atomic mass H = 1.008 amu
- 6.022×10^{23} He atoms in 4.003 g He
- atomic mass He = 4.003 amu
- 6.022×10^{23} S atoms in 32.07 g S
- atomic mass S = 32.07 amu

Figure 3.3 – One Mole of Several Substances



Example 3.2



Example 3.2

Consider titanium (Ti), the “space-age” metal discussed at the end of Chapter 1. Taking Avogadro’s number to be 6.022×10^{23} , calculate

- (a) the mass of a titanium atom.
- (b) the number of atoms in a ten-gram sample of the metal.
- (c) the number of protons in 0.1500 lb of titanium.

Strategy From the periodic table, the atomic mass of titanium is 47.87 amu. It follows that

$$6.022 \times 10^{23} \text{ Ti atoms} = 47.87 \text{ g Ti}$$

The relation yields the required conversion factor for (a) and (b). Also from the periodic table, we see that the atomic number for titanium is 22, the number of protons in an atom of titanium.

Example 3.2 (cont'd)



SOLUTION

$$(a) \text{ mass of Ti atom} = 1 \text{ Ti atom} \times \frac{47.87 \text{ g Ti}}{6.022 \times 10^{23} \text{ Ti atoms}} = 7.949 \times 10^{-23} \text{ g}$$

$$(b) \text{ no. of Ti atoms} = 10.00 \text{ g} \times \frac{6.022 \times 10^{23} \text{ Ti atoms}}{47.87 \text{ g Ti}} = 1.258 \times 10^{23} \text{ atoms}$$

(c) First, change the given mass of Ti (0.1500 lb) to grams:

$$0.1500 \text{ lb} \times \frac{453.6 \text{ g}}{1 \text{ lb}} = 68.04 \text{ g}$$

$$\begin{aligned} \text{no. of protons} &= 68.04 \text{ g} \times \frac{6.022 \times 10^{23} \text{ Ti atoms}}{47.87 \text{ g Ti}} \times \frac{22 \text{ protons}}{1 \text{ atom}} \\ &= 1.883 \times 10^{25} \text{ protons} \end{aligned}$$

Reality Check Because atoms are so tiny, we expect their mass to be very small: 7.949×10^{-23} g sounds reasonable. Conversely, it takes a lot of atoms, in this case 1.258×10^{23} , to weigh ten grams.



Ex 3-2 : Consider titanium Ti atomic mass : 47.87 amu

a) The mass of *a* titanium atom

b) The number of atoms in a 10.00g sample of Ti

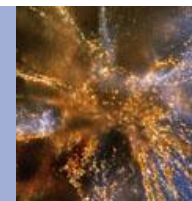
- a) Ti atom = 47.87g

$$1Ti \text{ atom} \times \frac{47.87 \text{ gTi}}{6.022 \times 10^{23} \text{ atoms}} = 7.949 \times 10^{-23} \text{ g}$$

- b)

$$10.00\text{g} \times \frac{6.022 \times 10^{23} \text{ atoms}}{47.87 \text{ gTi}} = 1.258 \times 10^{23} \text{ atoms}$$

§ 3-2 The Mole. (mol)



A mole represents 6.022×10^{23} items. (atoms or molecules)

- 1 mole H atoms = 6.022×10^{23} H atoms
- 1 mole O atoms = 6.022×10^{23} O atoms
- 1 mole H₂O molecules = 6.022×10^{23} H₂O

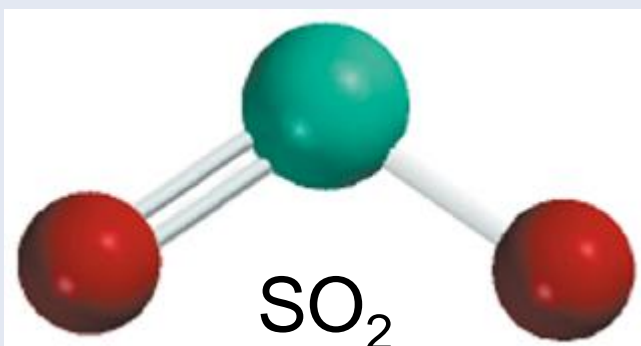
Molar mass (MM) :

- The Molar mass (MM) , in grams per mole, is numerically equal to the sum of the masses (in amu) of the atoms in the formula.

Formula	Sum of atomic masses	Molar mass ,MM
O	16.00amu	16.00g/mole
O ₂	2x16.00=32.00amu	32.00 g/ mole
H ₂ O	2(1.008)+16.00=18.02	18.02g/mole
NaCl	22.99+35.45=58.44	58.44 g/ mole

- Notice that the formula of a substance must be known to find its molar mass

Molecular mass

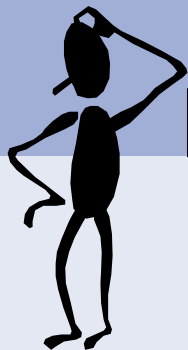


$$\begin{array}{r} 1\text{S} \qquad 32.07 \text{ amu} \\ 2\text{O} \qquad + 2 \times 16.00 \text{ amu} \\ \hline \text{SO}_2 \qquad 64.07 \text{ amu} \end{array}$$

For any molecule
molecular mass (amu) = molar mass (grams)

$$1 \text{ molecule SO}_2 = 64.07 \text{ amu}$$

$$1 \text{ mole SO}_2 = 64.07 \text{ g SO}_2$$



Do You Understand Molecular Mass?



How many H atoms are in 72.5 g of C_3H_8O ?

$$1 \text{ mol } C_3H_8O = (3 \times 12) + (8 \times 1) + 16 = 60 \text{ g } C_3H_8O$$

$$1 \text{ mol } C_3H_8O \text{ molecules} = 8 \text{ mol H atoms}$$

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

$$72.5 \text{ g } C_3H_8O \times \frac{1 \text{ mol } C_3H_8O}{60 \text{ g } C_3H_8O} \times \frac{8 \text{ mol H atoms}}{1 \text{ mol } C_3H_8O} \times \frac{6.022 \times 10^{23} \text{ H atoms}}{1 \text{ mol H atoms}} =$$

$$5.82 \times 10^{24} \text{ atoms H}$$

The Significance of the Mole



- In the laboratory, substances are weighed on balances, in units of grams
- The mole allows us to relate the number of grams of a substance to the number of atoms or molecules of a substance

Mole-Gram Conversions



- $m = MM \times n$
 - $m = \text{mass}$
 - $MM = \text{molar mass}$
 - $n = \text{number of moles}$



Ex 3-3 : Acetylsalicylic acid Aspirin 乙醯水楊酸 $C_9H_8O_4$

- a) What is the mass in grams of 0.509 mole of acetylsalicylic acid ?
- b) How many moles of $C_9H_8O_4$ are in a one gram sample of aspirin that contains 91.6 % by mass of acetylsalicylic acid ?

$$(a) C_9H_8O_4 Mw = 9 \times (12.01) + 8 \times (1.008) + 4 \times 16.00 = 180.15 \text{ g/mole}$$

$$0.509 \text{ mol} \times \frac{180.15 \text{ g}}{1 \text{ mol}} = 91.7 \text{ g}$$

$$(b) 1.00 \text{ g} \times 0.916 \times \frac{1 \text{ mol}}{180.15 \text{ g}} = 5.08 \times 10^{-3} \text{ mole}$$

Chemical Formulas



- In chapter 2, we learned that the chemical formula tells us the number of atoms of each element in a compound, whether that is a molecular compound or an ionic compound
- We can now combine that knowledge with the knowledge of molar mass to begin relating elements by mass

3.3 Mass Relations in Chemical Formulas



1. Percent composition from formula

- The percent composition of a compound is stated as the number of grams of each element in 100 g of the compound
- By knowing the formula, the mass percent of each element can be readily calculated



Ex 3.4. Metallic iron is most often extracted from hematite ore, which consists of iron (III) oxide mixed with impurities such as silicon dioxide, SiO_2 .

a). What are the mass percent of iron and oxygen in iron(III) oxide?

b). How many grams of iron can be extracted from one kilogram of Fe_2O_3 ?

c). How many metric tons of hematite ore, 66.4% Fe_2O_3 , must be processed to produce one kilogram of iron?

Sol

$$(a) \text{Fe}_2\text{O}_3 = 2 \times (55.85 \text{ g/mol}) + 3 \times (16.00 \text{ g/mol}) = 159.7 \text{ g}$$

$$\% \text{Fe} = \frac{111.7 \text{ g}}{159 \text{ g}} \times 100\% = 69.94$$

$$\% \text{O} = 100.0 - 69.94 = 3.06$$

$$(b) 1.000 \times 10^3 \text{ Fe}_2\text{O}_3 \times \frac{111.7 \text{ gFe}}{159.7 \text{ gFe}_2\text{O}_3} = 699.4 \text{ gFe}$$

$$(c) 1.00 \text{ KgFe} \times \frac{158.7 \text{ g}}{111.7 \text{ g}} \times \frac{100.0 \text{ g}}{66.4 \text{ gFe}_2\text{O}_3} \times \frac{1 \text{ metric ton}}{10^3 \text{ kg}}$$

$$= 2.14 \times 10^{-3} \text{ metric ton}$$

Chemical Analysis



- Experimentation can give data that lead to the determination of the formula of a compound
 - Masses of elements in the compound
 - Mass percents of elements in the compound
 - Masses of products obtained from the reaction of a weighed sample of the compound

2. Simplest Formula from Chemical Analysis



- Often, the formula is not known, but data from chemical analysis is known
 - Amount of each element in grams
 - Can be used to determine the simplest formula
 - Smallest whole-number ratio of atoms in a compound
 - H_2O is the simplest formula for water
 - H_2O_2 is the molecular formula for HO

Example 3.5 – Simplest Formula from Masses of Elements



Example 3.5 A 25.00-g sample of an orange compound contains 6.64 g of potassium, 8.84 g of chromium, and 9.52 g of oxygen. Find the simplest formula.

Strategy First (1), convert the masses of the three elements to moles. Knowing the number of moles (n) of K, Cr, and O, you can then (2) calculate the mole ratios. Finally (3), equate the mole ratio to the atom ratio, which gives you the simplest formula.

SOLUTION

$$(1) n_{\text{K}} = 6.64 \text{ g K} \times \frac{1 \text{ mol K}}{39.10 \text{ g K}} = 0.170 \text{ mol K}$$

$$n_{\text{Cr}} = 8.84 \text{ g Cr} \times \frac{1 \text{ mol Cr}}{52.00 \text{ g Cr}} = 0.170 \text{ mol Cr}$$

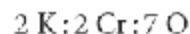
$$n_{\text{O}} = 9.52 \text{ g O} \times \frac{1 \text{ mol O}}{16.00 \text{ g O}} = 0.595 \text{ mol O}$$

(2) To find the mole ratios, divide by the smallest number, 0.170 mol K:

$$\frac{0.170 \text{ mol Cr}}{0.170 \text{ mol K}} = \frac{1.00 \text{ mol Cr}}{1 \text{ mol K}} \quad \frac{0.595 \text{ mol O}}{0.170 \text{ mol K}} = \frac{3.50 \text{ mol O}}{1 \text{ mol K}}$$

The mole ratio is 1 mol of K:1 mol of Cr:3.50 mol of O.

(3) As pointed out earlier, the mole ratio is the same as the atom ratio. To find the simplest whole-number atom ratio, multiply throughout by 2:



The simplest formula of the orange compound is $\text{K}_2\text{Cr}_2\text{O}_7$.

Reality Check A mole ratio of 1.00 A:1.00 B:3.33 C would imply a formula $\text{A}_3\text{B}_3\text{C}_{10}$; if the mole ratio were 1.00 A:2.50 B:5.50 C, the formula would be $\text{A}_2\text{B}_5\text{C}_{11}$. In general, multiply through by the smallest whole number that will give integers for all the subscripts.



Ex 3-5 A 25.00g orange compound 含 6.64g potassium
K(39.10) 8.84g chromium Cr (52.00) , 9.52g oxygen O
(16.00) Find the simplest formula ?

- $K : Cr : O = \frac{6.64}{39.10} : \frac{8.84}{52.00} : \frac{9.52}{16.00}$
- $= 0.170 : 0.170 : 0.595 = 1.00 : 1.00 : 3.5$
- $= 2 : 2 : 7$
- $K_2Cr_2O_7$
- 或 : K佔26.6 % , Cr佔35.4 % , O佔38.0 %
- Basis : 取100g
- $K : Cr : O = \frac{26.6}{39.10} : \frac{35.4}{52.00} : \frac{38.0}{16.00}$
-
- $= 0.68 : 0.68 : 2.38 = 1 : 1 : 3.5$
-

Example 3.6 – Simplest Formula from Mass Percents



- When dealing with percentages, assume 100 g of the compound
- By doing so, the unitless percentage becomes a meaningful mass

Example 3.6

The compound that gives vinegar its sour taste is acetic acid, which contains the elements carbon, hydrogen, and oxygen. When 5.00 g of acetic acid are burned in air, 7.33 g of CO_2 and 3.00 g of water are obtained. What is the simplest formula of acetic acid?

Example 3.6 – Simplest Formula from Mass Percents (cont'd)



Strategy The first step (1) is to calculate the masses of C, H, and O in the 5.00-g sample. To do this note that all of the carbon has been converted to carbon dioxide. One mole of C (12.01 g) forms one mole of CO₂ (44.01 g). Hence to find the mass of carbon in 7.33 g of CO₂, you use the conversion factor:

$$12.01 \text{ g C} / 44.01 \text{ g CO}_2$$

By the same token, all the hydrogen ends up as water. Because there are two moles of H (2.016 g) in one mole of H₂O (18.02 g), the conversion factor is

$$2(1.008) \text{ g H} / 18.02 \text{ g H}_2\text{O}$$

The mass of oxygen in the sample cannot be found in a similar way because some of the oxygen in the products comes from the air required to burn the reactants. Instead we find the mass of oxygen by difference:

$$\text{mass O} = \text{mass of sample} - (\text{mass of C} + \text{mass of H})$$

Once the masses of the elements are obtained, it's all downhill; follow the same path as in Example 3.5.

Example 3.6 – Simplest Formula from Mass Percents (cont'd)



SOLUTION

(1) Find the mass of each element in the sample.

$$\text{mass C} = 7.33 \text{ g CO}_2 \times \frac{12.01 \text{ g C}}{44.01 \text{ g CO}_2} = 2.00 \text{ g C}$$

$$\text{mass H} = 3.00 \text{ g H}_2\text{O} \times \frac{2.016 \text{ g H}}{18.02 \text{ g H}_2\text{O}} = 0.336 \text{ g H}$$

$$\text{mass O} = 5.00 \text{ g sample} - 2.00 \text{ g C} - 0.336 \text{ g H} = 2.66 \text{ g O}$$

(2) Find the number of moles of each element.

$$n_{\text{C}} = 2.00 \text{ g C} \times \frac{1 \text{ mol C}}{12.01 \text{ g C}} = 0.167 \text{ mol C}$$

$$n_{\text{H}} = 0.336 \text{ g H} \times \frac{1 \text{ mol H}}{1.008 \text{ g H}} = 0.333 \text{ mol H}$$

$$n_{\text{O}} = 2.66 \text{ g O} \times \frac{1 \text{ mol O}}{16.00 \text{ g O}} = 0.166 \text{ mol O}$$

(3) Find the mole ratios and then the simplest formula.

$$\frac{0.167 \text{ mol C}}{0.166 \text{ mol O}} = \frac{1.01 \text{ mol C}}{1.00 \text{ mol O}} \quad \frac{0.333 \text{ mol H}}{0.166 \text{ mol O}} = \frac{2.01 \text{ mol H}}{1.00 \text{ mol O}}$$

Rounding off to whole numbers, the mole ratios are

$$1 \text{ mol C} : 2 \text{ mol H} : 1 \text{ mol O}$$

The simplest formula of acetic acid is CH_2O .



Ex 3-6 : The compound that gives vinegar its sour taste is acetic acid ,which contains the elements carbon, hydrogen and oxygen. When a sample of acetic acid is burned in air, What is the simplest formula of acetic acid ? 5.00g acetic acid \rightarrow 7.33g CO₂+3.00gH₂O(含C、 H、 O)

sol

$$(1)m(C) = 7.33 \times \frac{M_C}{M_{CO_2}} = 7.33 \times \frac{12.01}{44.01} = 2.00g \quad (2) 2.00 \times \frac{1}{12.01} = 0.167$$

$$m(H) = 3.0gH_2O \times \frac{2.016}{18.02} = 0.336g \quad 0.336 \times \frac{1}{1.008} = 0.333$$

$$M(O) = 5.00 - 2.00 - 0.336 = 2.66g \quad 2.66g \times \frac{1}{16.00} = 0.166$$

$$(3) \frac{0.167}{0.166} = \frac{1.01C}{1.00O} \quad \frac{0.333H}{0.166O} = \frac{2.01}{1.00}$$

$$\therefore 1molC : 2molH : 1molO = CH_2O$$

3. Molecular Formula from Simplest Formula



- The relationship between simplest and molecular formula is a whole number
- The whole number relates the molecular mass to the mass of the simplest formula as well

Example 3.7



Example 3.7

The molar mass of acetic acid, as determined with a mass spectrometer, is about 60 g/mol. Using that information along with the simplest formula found in Example 3.6, determine the molecular formula of acetic acid.

Strategy Calculate the molar mass corresponding to the simplest formula, CH₂O. Then find the multiple by dividing the actual molar mass, 60 g/mol, by the molar mass of CH₂O.

SOLUTION

$$\text{MM CH}_2\text{O} = 12.01 \text{ g/mol} + 2(1.008 \text{ g/mol}) + 16.00 \text{ g/mol} = 30.03 \text{ g/mol}$$

The ratio of the actual molar mass, 60 g/mol, to that of CH₂O is

$$\frac{60 \text{ g/mol}}{30.03 \text{ g/mol}} = 2; \quad \text{molecular formula} = \text{C}_2\text{H}_4\text{O}_2$$

§ 3-4 Mass relations in reactions



1. Writing and balancing chemical equations

- (1) Any calculation involving a reaction must be based on the balanced equation for that reaction.
- (2) You cannot write an equation unless you know what happens in the reaction that it represents.

Balancing Chemical Equations



1. Write the **correct** formula(s) for the reactants on the left side and the **correct** formula(s) for the product(s) on the right side of the equation.

Ethane reacts with oxygen to form carbon dioxide and water



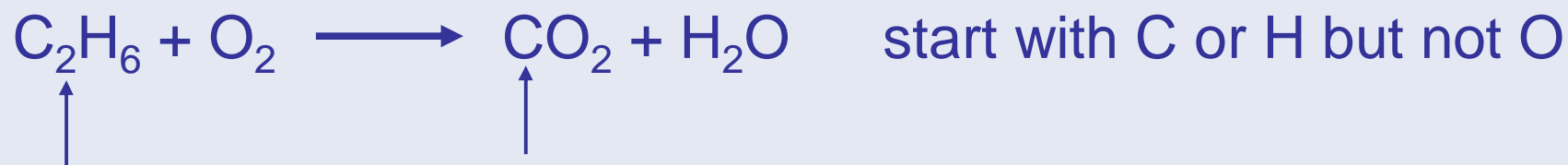
2. Change the numbers in front of the formulas (***coefficients***) to make the number of atoms of each element the same on both sides of the equation. Do not change the subscripts.



Balancing Chemical Equations



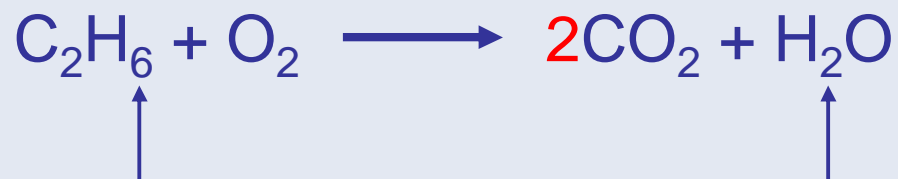
3. Start by balancing those elements that appear in only one reactant and one product.



2 carbon
on left

1 carbon
on right

multiply CO_2 by **2**



6 hydrogen
on left

2 hydrogen
on right

multiply H_2O by **3**



Balancing Chemical Equations



5. Check to make sure that you have the same number of each type of atom on both sides of the equation.



4 C (2 x 2)

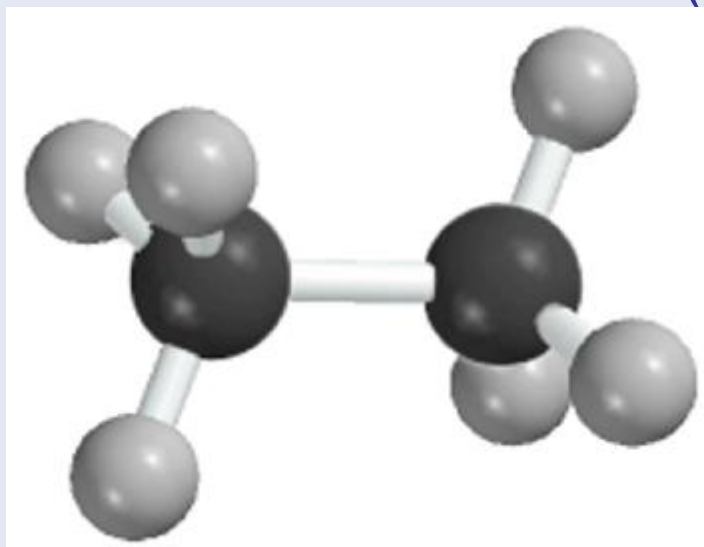
4 C

14 O (7 x 2)

14 O (4 x 2 + 6)

12 H (2 x 6)

12 H (6 x 2)



<u>Reactants</u>	<u>Products</u>
4 C	4 C
12 H	12 H
14 O	14 O

How are Equations Written?



- We must know the reactants and the products for a reaction for which an equation is to be written
 - It is often necessary to do an **experiment** and an analysis to determine the products of a reaction
 - Determining the products is often time consuming and difficult

Writing Chemical Equations



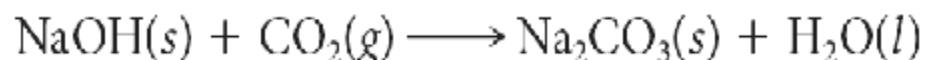
1. Write a **skeleton** equation for the reaction.
2. Indicate the **physical state** of each reactant and product.
3. Balance the equation
 - Only the **coefficients** can be changed; subscripts are fixed by chemical nature of the reactants and products
 - It is best to balance atoms that appear only **once on each side** of the equation first

Example 3.8

Crystals of sodium hydroxide (lye) react with carbon dioxide from air to form a colorless liquid, water, and a white powder, sodium carbonate, which is commonly added to detergents as a softening agent. Write a balanced equation for this chemical reaction.

Strategy To translate names into formulas, recall the discussion in Section 2.6, Chapter 2. The physical states are given or implied. To balance the equation, you could start with either sodium or hydrogen.

SOLUTION The skeleton equation is



Because there are two Na atoms on the right, a coefficient of 2 is written in front of NaOH:

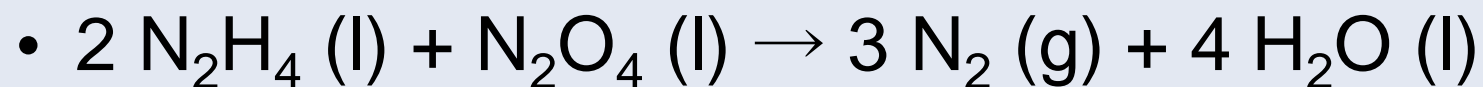


Careful inspection shows that all atoms are now balanced. There are two Na atoms, four O atoms, two H atoms, and one C atom on both sides of the equation.

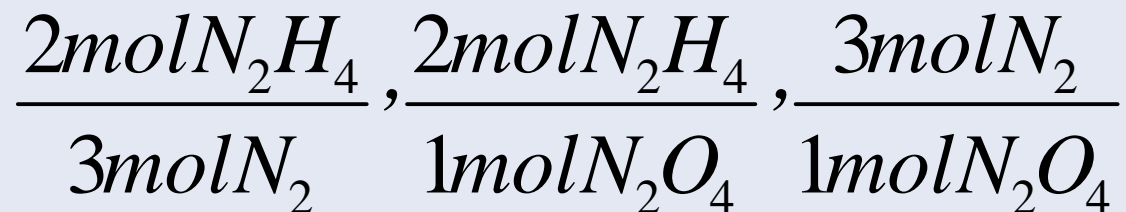
Mass Relations from Equations



- The coefficients of a balanced equation represent the numbers of moles of reactants and products



The coefficients of a balanced equation represent numbers of moles of reactants and products



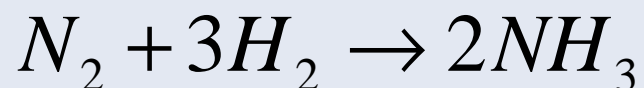
How many moles of hydrazine 肼 were required to form 1.8 mol of elemental nitrogen, the conversion would be?

$$n_{\text{N}_2\text{H}_4} = 1.80\text{molN}_2 \times \frac{2\text{molN}_2\text{H}_4}{3\text{molN}_2} = 1.20\text{molN}_2\text{H}_4$$



Ex 3-9 : Ammonia used to make fertilizers for lawns and gardens is made by reacting nitrogen with hydrogen :

- The number of moles of ammonia formed when 1.34mol of N_2 reacts.
- The mass in grams of N_2 required to form 1.00×10^3 g NH_3
- The number of molecules of ammonia formed When 1.34g of H_2 reacts.



$$n_{NH_3} = 1.34 \text{ mol } N_2 \times \frac{2 \text{ mol } NH_3}{1 \text{ mol } N_2} = 2.68 \text{ mol } NH_3$$

$$\text{mass } N_2 = 1.00 \times 10^3 \text{ g } NH_3 \times \frac{1 \text{ mol}}{17.03 \text{ g}} \times \frac{1 \text{ mol } N_2}{2 \text{ mole } NH_3} \times \frac{28.02 \text{ g } N_2}{1 \text{ mol } N_2} = 823 \text{ g } N_2$$

$$\begin{aligned} \text{no. molecules } NH_3 &= 1.34 \text{ g} \times \frac{1 \text{ mol } H_2}{2.016 \text{ g } H_2} \times \frac{2 \text{ mol } NH_3}{3 \text{ mol } H_2} \times \frac{6.022 \times 10^{23}}{1 \text{ mol } NH_3} \\ &= 2.67 \times 10^{23} \text{ molecules } N H_3 \end{aligned}$$

Example 3.9

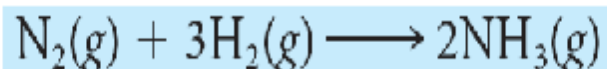
Graded

Ammonia is used to make fertilizers for lawns and gardens by reacting nitrogen gas with hydrogen gas.

- * (a) Write a balanced equation with smallest whole-number coefficients for this reaction.
- * (b) How many moles of ammonia are formed when 1.34 mol of nitrogen react?
- ** (c) How many grams of hydrogen are required to produce 2.75×10^3 g of ammonia?
- ** (d) How many molecules of ammonia are formed when 2.92 g of hydrogen react?
- *** (e) How many grams of ammonia are produced when 15.0 L of air (79% by volume nitrogen) react with an excess of hydrogen? The density of nitrogen at the conditions of the reaction is 1.25 g/L.

SOLUTION

(a) The equation for the reaction is



(b) The reaction gives you the stoichiometric mole ratio: 2 moles NH_3 /1 mole N_2 . Thus,

$$n_{\text{NH}_3} = 1.34 \text{ mol N}_2 \times \frac{2 \text{ mol NH}_3}{1 \text{ mol N}_2} = 2.68 \text{ mol NH}_3$$

(c) Here we follow the scheme

$$m_{\text{NH}_3} \xrightarrow{\text{MM}} n_{\text{NH}_3} \xrightarrow{\text{ratio}} n_{\text{H}_2} \xrightarrow{\text{MM}} m_{\text{H}_2}$$

$$\text{mass H}_2 = 2.75 \times 10^3 \text{ g NH}_3 \times \frac{1 \text{ mol NH}_3}{17.03 \text{ g NH}_3} \times \frac{3 \text{ mol H}_2}{2 \text{ mol NH}_3} \times \frac{2.016 \text{ g H}_2}{1 \text{ mol H}_2} = 488 \text{ g H}_2$$

(d) We add the Avogadro conversion factor N_A to the scheme:

$$m_{\text{H}_2} \xrightarrow{\text{MM}} n_{\text{H}_2} \xrightarrow{\text{ratio}} n_{\text{NH}_3} \xrightarrow{N_A} \text{molecules NH}_3$$

$$\text{molecules NH}_3 = 2.92 \text{ g H}_2 \times \frac{1 \text{ mol H}_2}{2.016 \text{ g H}_2} \times \frac{2 \text{ mol NH}_3}{3 \text{ mol H}_2} \times \frac{6.022 \times 10^{23} \text{ molecules}}{1 \text{ mol NH}_3}$$

$$= 5.81 \times 10^{23} \text{ molecules}$$

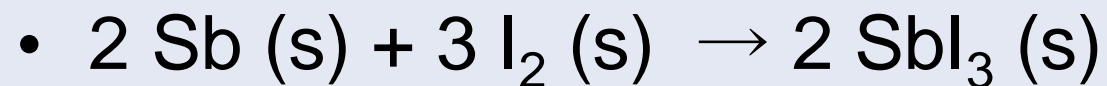
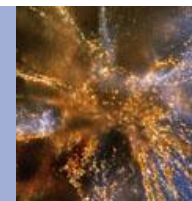
(e) We first find the mass of nitrogen in air and then proceed using a scheme similar to those above.

$$m_{\text{N}_2} \xrightarrow{\text{MM}} n_{\text{N}_2} \xrightarrow{\text{ratio}} n_{\text{NH}_3} \xrightarrow{\text{MM}} m_{\text{NH}_3}$$

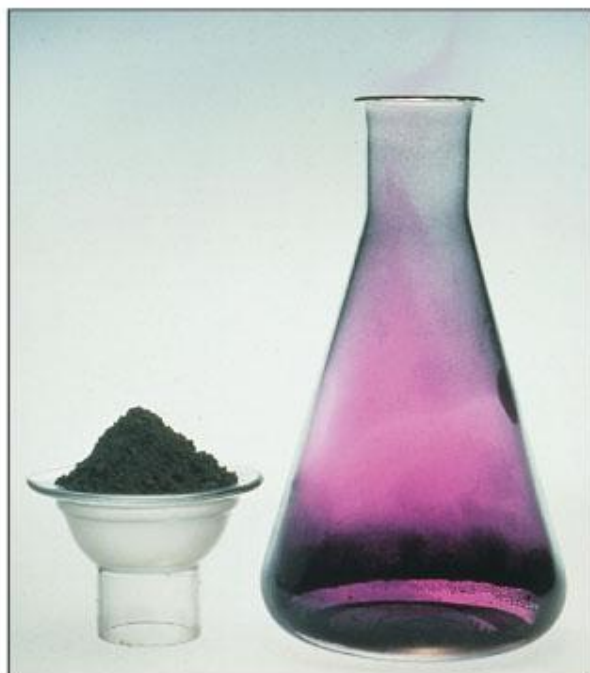
$$\text{mass N}_2 = 15.0 \text{ L air} \times \frac{79 \text{ L N}_2}{100 \text{ L air}} \times \frac{1.25 \text{ g N}_2}{1 \text{ L N}_2} = 14.8 \text{ g N}_2$$

$$m_{\text{NH}_3} = 14.8 \text{ g N}_2 \times \frac{1 \text{ mol N}_2}{28.02 \text{ g N}_2} \times \frac{2 \text{ mol NH}_3}{1 \text{ mol N}_2} \times \frac{17.03 \text{ g NH}_3}{1 \text{ mol NH}_3} = 18 \text{ g NH}_3$$

3 Limiting Reactant and Theoretical Yield

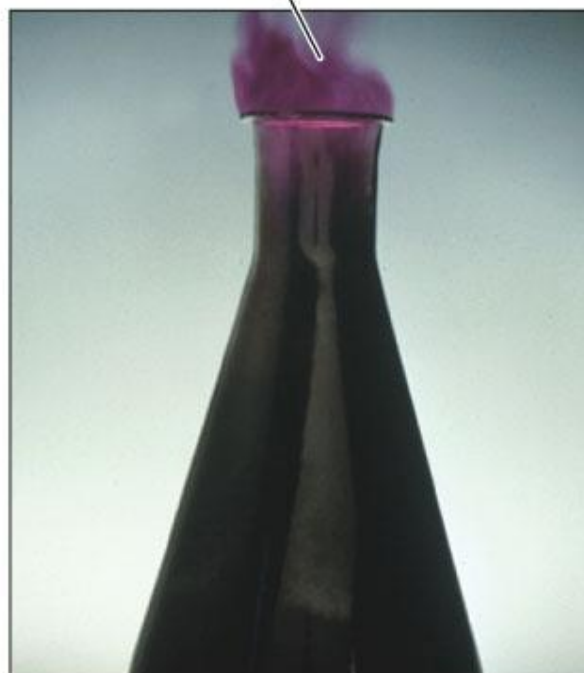


1 When antimony (dark gray powder) comes in contact with iodine (violet vapor)...



The Reactants

2 ...a vigorous reaction takes place.



The Reaction

3 The product is SbI_3 , a red solid.



The Product

Interpreting by Mass



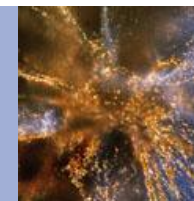
- Reactants
 - Two mole Sb (243.6 g)
 - Three moles I₂ (761.4 g)
 - Two moles SbI₃ (1005.0 g)
- All of the reactants are converted to product
- $2 \text{ Sb (s)} + 3 \text{ I}_2 \text{ (s)} \rightarrow 2 \text{ SbI}_3 \text{ (s)}$

In the Laboratory

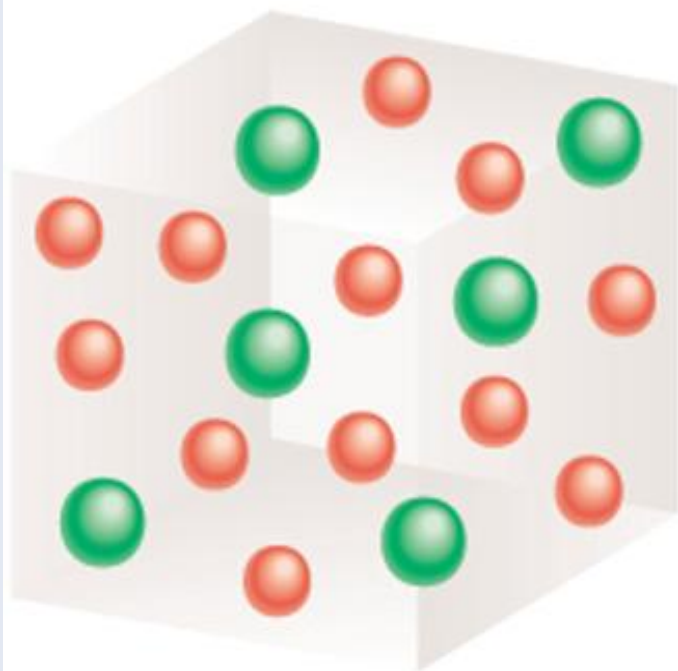



- Reactants are usually not mixed in exact ratios
- An excess of one reactant is often used
 - Usually the less (or least) expensive reactant
 - One reactant will then limit the amount of product that will form


(Limiting Reagents)



Before reaction has started

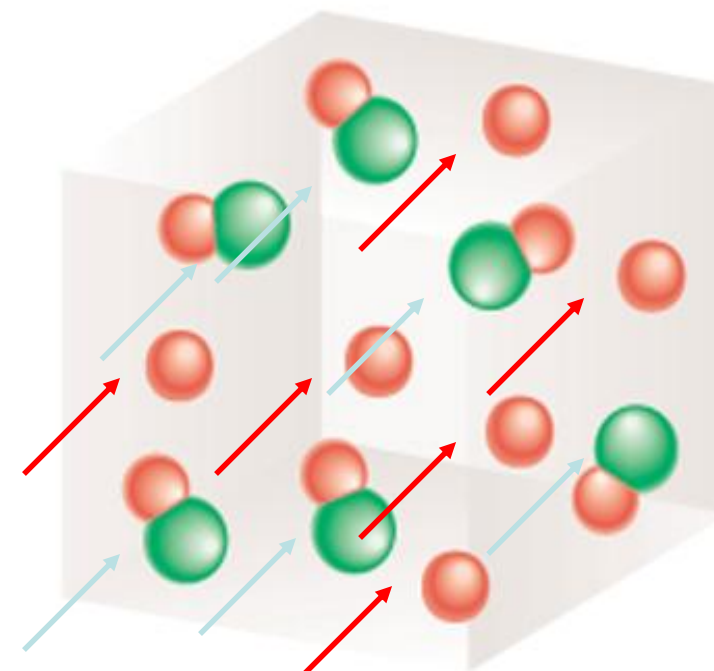


 Limiting reagent

 Excess reagent



After reaction is complete



6 red leftover

Sb-I₂ with a limiting reactant



- Suppose the mixture is
 - 3.00 mol Sb
 - 3.00 mol I₂
- In this case
 - 1.00 mol Sb will be left over
 - 2.00 mol of Sb will be used
 - React with 3.00 mol I₂
 - Form 2.00 mol SbI₃
- $2 \text{ Sb (s)} + 3 \text{ I}_2 \text{ (s)} \rightarrow 2 \text{ SbI}_3 \text{ (s)}$

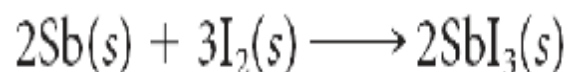
Approach to Limiting Reactant Problems



1. Calculate the amount of product that will form if the first reactant were **completely consumed**.
2. Repeat the calculation for the second reactant in the same way.
3. Choose the **smaller amount of product** and relate it to the reactant that produced it. This is the limiting reactant and the resulting amount of product is the ***theoretical yield***.
4. From the theoretical yield, determine how much of the reactant in excess is used, and subtract from the starting amount.

Example 3.10

Consider the reaction



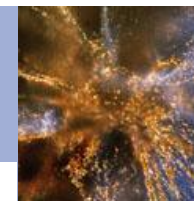
Determine the limiting reactant and the theoretical yield when

- (a) 1.20 mol of Sb and 2.40 mol of I_2 are mixed.
- (b) 1.20 g of Sb and 2.40 g of I_2 are mixed. What mass of excess reactant is left when the reaction is complete?

Strategy Follow the four steps outlined above. In steps (1) and (2), follow the strategy described in Example 3.9 to calculate the amount of product formed. In (a), a simple one-step conversion is required; in (b), the path is longer because you have to go from mass of reactant to mass of product. To find the mass of reactant left over in (b), calculate how much is required to give the theoretical yield of product. Subtract that from the starting amount to find the amount left.



Example 3.10



SOLUTION

(a) (1) n_{SbI_3} from Sb = $1.20 \text{ mol Sb} \times \frac{2 \text{ mol SbI}_3}{2 \text{ mol Sb}} = 1.20 \text{ mol SbI}_3$

(2) n_{SbI_3} from $\text{I}_2 = 2.40 \text{ mol I}_2 \times \frac{2 \text{ mol SbI}_3}{3 \text{ mol I}_2} = 1.60 \text{ mol SbI}_3$

(3) Because **1.20 mol** is the smaller amount of product, that is the theoretical yield of SbI_3 . This amount of SbI_3 is produced by the antimony, so **Sb is the limiting reactant.**

(b) (1) mass of SbI_3 from Sb = $1.20 \text{ g Sb} \times \frac{1 \text{ mol Sb}}{121.8 \text{ g Sb}} \times \frac{2 \text{ mol SbI}_3}{2 \text{ mol Sb}} \times \frac{502.5 \text{ g SbI}_3}{1 \text{ mol SbI}_3}$
 $= 4.95 \text{ g SbI}_3$

(2) mass of SbI_3 from $\text{I}_2 = 2.40 \text{ g I}_2 \times \frac{1 \text{ mol I}_2}{253.8 \text{ g I}_2} \times \frac{2 \text{ mol SbI}_3}{3 \text{ mol I}_2} \times \frac{502.5 \text{ g SbI}_3}{1 \text{ mol SbI}_3}$
 $= 3.17 \text{ g SbI}_3$

(3) The reactant that yields the smaller amount (3.17 g) of SbI_3 is I_2 . Hence **I_2 is the limiting reactant.** The smaller amount, **3.17 g** of SbI_3 , is the theoretical yield.

(4) mass of Sb required = $3.17 \text{ g SbI}_3 \times \frac{121.8 \text{ g Sb}}{502.5 \text{ g SbI}_3} = 0.768 \text{ g Sb}$

mass of Sb left = $1.20 \text{ g} - 0.768 \text{ g} = \mathbf{0.43 \text{ g}}$

Experimental Yield



- Experimental yields are always lower than theoretical yields
 - Some product is lost to competing reactions
 - Some product is lost to handling
 - Some product may be lost in separating it from the reaction mixture
- The ***actual yield*** is the quantity of product you measure after you have done the reaction in the laboratory

Percent Yield

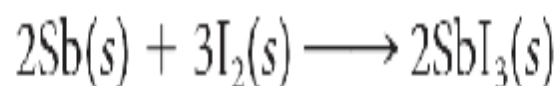


- The percent yield is defined as

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

Example 3.11

Consider again the reaction discussed in Example 3.10:



Suppose that in part (a) the percent yield is 78.2%. How many grams of SbI_3 are formed?

Strategy Use Equation 3.3 to find the number of moles of SbI_3 and then the mass in grams ($1 \text{ mol SbI}_3 = 502.5 \text{ g SbI}_3$).

SOLUTION

$$\text{experimental yield SbI}_3 = 1.20 \text{ mol SbI}_3 \times \frac{78.2}{100} \times \frac{502.5 \text{ g SbI}_3}{1 \text{ mol SbI}_3} = 472 \text{ g SbI}_3$$

Key Concepts



1. Relate the atomic mass of an element to isotopic masses and abundances.
2. Use Avogadro's number to calculate the mass of an atom or molecule (in grams).
3. Use molar mass to relate
 - Moles to mass of a substance
 - Molecular formula to simplest formula
4. Use the formula of a compound to find its percent composition or the equivalent

Key Concepts



5. Find the simplest formula of a compound from chemical analysis
6. Balance chemical equations by inspection
7. Use a balanced equation to
 - Relate masses of reactants and products
 - Find the limiting reactant, theoretical yield, and percent yield of a reaction.