Ch.3 Mass Relations in Chemistry Stoichiometry

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Ch.3 Mass Relations in Chemistry Stoichiometry

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.

§ 3-1 Atomic masses；the carbon -12 scale

The modern atomic mass scale is based on the most common isotope of carbon $^{12}_{6}C$. This isotope is assigned a mass of exactly 12 atomic mass units (amu).

mass of C–12 atom = 12 amu (exactly) 12.00 amu

Isotope: 原子有相同之原子序不同之質量數; $^{12}_{6}C, ^{13}_{6}C, ^{14}_{6}C$

H: 1.008 amu

He: 4.003 amu

Atomic masses are cited to four significant figures.

§ Atomic masses and isotopic abundance

Relative masses of individual atoms can be determined using a mass spectrometer 質譜儀

Process: 低壓下，氣態原子 or 分子離子化失去一個 or 多個電子生成氣態離子⇒(陽離子), 通過電位 500 ~ 2000V 之加速板，加速進入磁場，其會產生偏移，其偏斜與 e/m 有關。因此具有相等電荷但不同質量的離子即可分離，故可以測出同位素的相對含量（**isotopic abundance**）. 同種原子較輕之原子偏移較大，重的偏移較小, 較輕之同位素先偵測到.

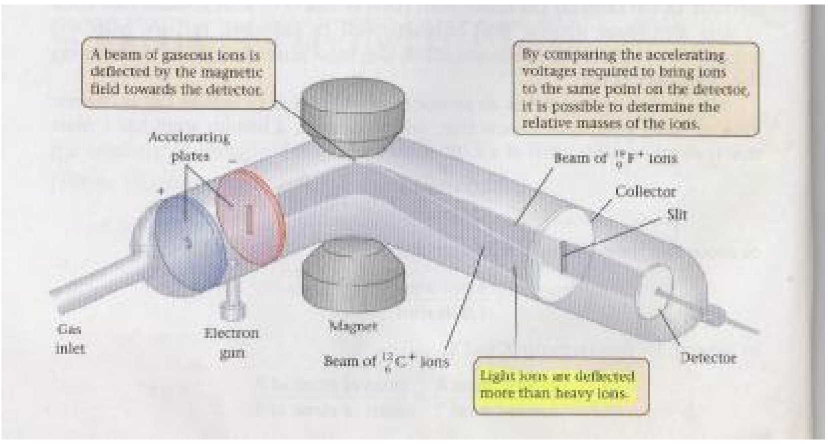

Fig. 3.1 The mass spectrometer

吸收波面積↑⇒含 量↑

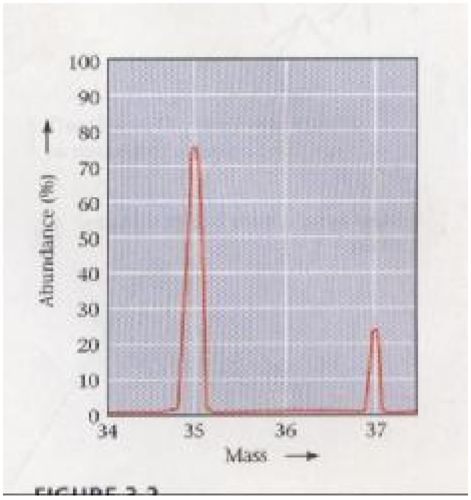

Figure 3.2 Mass spectrum of chlorine.

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

Cl atomic mass = $34.97\times 75.53\% + 36.97\times 24.47\% = 35.46 amu$

Ex 3.1: Bromine is a red-orange liquid with an average atomic mass of 79.90 amu. Its name is derived from the Greek word bromos, which means stench. It has two naturally occurring isotopes: Br-79 (78.92 amu), Br-81 (80.92 amu). What is the abundance of the heavier isotope？

設：Br-81 含量 x　　Br-79 佔 1-x

$$\therefore \quad 79.90 = 78.92 \times (1 - x) + 80.92 \times x$$
$$79.90 = 78.92 + 2.00\, x$$
$$x = 0.490$$

∴ Br-81 佔 49.0%

§ Masses of individual atoms; Avogadro’s number

Avogadro’s number

$N_A = 6.022 \times 10^{23}$ (four significant figures)

A sample of any element with a mass in grams equal to its atomic mass contains the same number of atoms, N_A, regardless of the identity of the element.

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

Ex 3.2: Consider titanium (Ti), the “space-age” metal. Taking Avogadro’s number to be $6.022\text{x}10^{23}$, calculate:
a) the mass of ***a*** titanium atom.
b) the number of atoms in a 10.00g sample of the metal.
c) the number of protons in 0.1500 lb of titanium.

Ans: Atomic mass of Ti：47.87 amu

a) $6.022\times10^{23} \times 10^{23}$ Ti atoms = 47.87 g

$$\therefore \quad 1 : 6.022\times10^{23} = x : 47.87$$
$$x = 7.949 \times 10^{-23}\ \text{g}$$

b) $\dfrac{10.00}{47.87} \times 6.022\times10^{23} = 1.258 \times 10^{23}$ atoms Ti atom = 47.87g

c) $0.1500\ \text{lb} \times \dfrac{453.6\ \text{g}}{1\ \text{lb}} = 68.04\ \text{g}$

$$\frac{68.04}{47.87} \times 6.022\times10^{23} \times \frac{22\ \text{protons}}{1\ \text{atom}} = 1.833 \times 10^{25}\ \text{protons}$$

§ 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

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	16.00 amu	16.00 g/mol
O_2	$2\times 16.00 = 32.00 amu$	32.00 g/mol
H_2O	$2(1.008)+16.00=18.02 amu$	18.02 g/mol
$NaCl$	$22.99+35.45=58.44 amu$	58.44 g/mol

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

§ Mole-gram Conversions

m = mass in grams

$m = MM \times n$ MM = molar mass g/mol

n = amount in moles

Ex 3.3: Acetylsalicylic acid, $C_9H_8O_4$, **is the active ingredient of aspirin**

$C_9H_8O_4$ Acetylsalicylic acid $\Rightarrow$ Aspirin
乙醯水楊酸

a) What is the mass in grams of 0.509 mole of acetylsalicylic acid？
b) A 1.00g sample of aspirin contains 75.2 % by mass of $C_9H_8O_4$. How many moles of acetylsalicylic acid are in the sample？
c) How many molecules of $C_9H_8O_4$ are there in 12.00 g of acetylsalicylic acid？How many carbon atoms？

Ans:

$a)\ C_9H_8O_4$ 之 $MM = 9\times(12.01)+8\times(1.008)+4\times(16.00)=180.15\ {}^{g}\!/_{mol}$

$m = 0.509 \times 180.15 = 91.7\ g$

b) $1.00\times 75.2\% \div 180.15 = 4.17 \times 10^{-3}\ mol$

$c)\ \frac{12.00}{180.15} \times 6.022\times 10^{23} = 4.011 \times 10^{22}\ C_9H_8O_4$ molecules

4.011×10^{22} molecules $\times \frac{9\ \text{C atoms}}{1\ \text{molecule}} = 3.610 \times 10^{23}$ C atoms

§ 3-3 Mass relations in chemical formulas 質量與化學式關係

應用：1. The formula for a compound can be used to determine the mass percents of the elements present. 由各元素所佔質量百分比計算之.

2. Simplest formula. ⇒ 簡式 or 實驗式 (empirical formula)

3. 由分子量 ⇒ 分子式 (實驗式)$_n$ = 分子式

§ Percent Composition from formula

The percent composition of a compound is specified by citing the mass percents of the elements present.

H_2O： hydrogen: 11.19g oxygen: 88.81g

H = (11.19/100.00g) × 100% = 11.19 %

O =(88.81g/100.00g) × 100 % = 88.81 %

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?

Ans:

$a)\ MM_{Fe_2O_3} = 2 \times (55.85) + 3 \times (16.00) = 159.70\ g/mol$

$Fe\ (\%) = (111.70/159.70) \times 100 = 69.94\ \%$

$O\ (\%) = (48.00/159.70) \times 100 = 30.06\ \%$

$b)\ 1.00 \times 10^3 \times 69.94\ \% = 699.4\ g$

$c)\ 1.000/69.94\% = 1.430\ kg\ Fe_2O_3$

$1.430/66.4\% = 2.15\ kg$ hematite ore $= 2.15 \times 10^{-3}$ ton hematite ore

簡式可由下列不同方法獲知

- the masses of the elements in a weighted sample of the compound. (Ex 3.5)
- the mass percents of the elements in the compound.
- the mass of products obtained by reaction of a weighted sample of the compound. 由化學反應得知 (Ex 3.6)

Ex 3.5: A 25.00g sample of an orange compound contains 6.64 g of potassium, (K : 39.10 $g/mole$), 8.84 g of chromium (Cr:52.00 $g/mole$) and 9.52 g of oxygen (O:16.00 $g/mole$). Find the simplest formula？

Ans:

$$n_K : n_{Cr} : n_O = \frac{6.64}{39.10} : \frac{8.844}{52.00} : \frac{9.52}{16.00}$$

$$= 0.170 : 0.170 : 0.595$$

$$= 1.00 : 1.00 : 3.50$$

通分得整數比

$$= 2 : 2 : 7$$

$\therefore K_2Cr_2O_7$ 重鉻酸鉀

或：例: K 佔 26.6 %; Cr 佔 35.4 %; O 佔 38.0 %

$\Rightarrow$ Basis：取 100g

$$n_K : n_{Cr} : n_O = \frac{26.6}{39.10} : \frac{35.4}{52.00} : \frac{38.0}{16.00}$$

$$= 0.680 : 0.680 : 2.38$$

$$= 1.00 : 1.00 : 3.50$$

通分得整數比

$$= 2 : 2 : 7$$

$\therefore K_2Cr_2O_7$

Ex 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 3.00g of water are obtained. What is the simplest formula of acetic acid？

$$5.00\text{g acetic acid} \xrightarrow{\vee} 7.33\text{g } CO_2(\text{g}) + 3.00g\ H_2O(\text{g})$$

Ans:

$$\text{C 燃燒} \rightarrow CO_2(\text{g})$$
$$\text{H 燃燒} \rightarrow H_2O(\text{g})$$

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

$$m\ (H) = 3.00 \times \frac{M_{H_2}}{M_{H_2O}} = 3.00 \times \frac{2.02}{18.02} = 0.336\ g$$

$$m\ (O) = 5.00 - 2.00 - 0.336 = 2.664\ g$$

$$n_C : n_H : n_O = \frac{2.00}{12.01} : \frac{0.336}{1.008} : \frac{2.664}{16.00}$$
$$= 0.167 : 0.333 : 0.167$$
$$= 1 : 2 : 1$$

$$\therefore \text{簡式} \Rightarrow CH_2O$$

§ Molecular formula from simplest formula

(simplest formula) × n = molecular formula

n 由分子量決定

Ex 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. Acetic acid molar mass = 60 $^{g}/_{mol}$

Ans: 接續 Ex 3.6 求分子式

$$(CH_2O) \times n = 60$$
$$(12.01 + 2 \times 1.008 + 16.00) \times n = 60$$
$$n = 2$$
$$\therefore\ Aceticacid:\ C_2H_4O_2 \Rightarrow CH_3COOH\ (\text{示性式})$$

§ 3-4 Mass relations in reactions

§ Writing and balancing chemical equations

Any calculation involving a reaction must be based on the balanced equation for that reaction.（原子不滅；質能不滅）

例：太空船，使用 $N_2H_4(\mathbf{l})$ 聯胺及 $N_2O_4(\mathbf{l})$ 爲燃料生成 $N_2(g)$ 及 $H_2O(g)$

1. $N_2H_4 + N_2O_4 \rightarrow N_2 + H_2O$

   $reactants$ (左)　　products (右)

2. 標示狀態：

   $N_2H_4(\mathbf{l}) + N_2O_4(\mathbf{l}) \rightarrow N_2(g) + H_2O(g)$

3. Balance:

   O:　左: 4　　右：1 × 4

   $N_2H_4(\mathbf{l}) + N_2O_4(\mathbf{l}) \rightarrow N_2(g) + 4H_2O(g)$

   H:　左: 4×2　　右：4×2 =8

   $2N_2H_4(\mathbf{l}) + N_2O_4(\mathbf{l}) \rightarrow N_2(g) + 4H_2O(g)$

   N:　左: 2×2 + 2 = 6　　右：2 × 3

   $2N_2H_4(\mathbf{l}) + N_2O_4(\mathbf{l}) \rightarrow 3N_2(g) + 4H_2O(g)$

Ex 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 balance equation for this chemical reaction.

Ans:

$NaOH(s) + CO_2(g) \rightarrow Na_2CO_3(s) + H_2O(\mathbf{l})$

Na:　左: 1 × 2　　右: 2

$2NaOH(s) + CO_2(g) \rightarrow Na_2CO_3(s) + H_2O(\mathbf{l})$

H:　左: 2　　右: 2　　ok

C:　左: 1　　右: 1　　ok

O:　左: 2 + 2 = 4　　右: 3 + 1 = 4　　ok

$\therefore\ 2NaOH(s) + CO_2(g) \rightarrow Na_2CO_3(s) + H_2O(\mathbf{l})$

§ Mass relations from equations

$$2N_2H_4(\mathbf{l}) + N_2O_4(\mathbf{l}) \longrightarrow 3N_2(g) + 4H_2O(g)$$

2 mole	1 mole	3 mole	4 mole
2 分子	1 分子	3 分子	4 分子
$2N_A$	$1N_A$	$3N_A$	$4N_A$

Ex 3.9: Ammonia used to make fertilizers for lawns and gardens is made by reacting nitrogen with hydrogen ：

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 reacts.

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 excess of hydrogen？ The density of nitrogen at the conditions of the reaction is 1.25 g/L.

Ans:

a) $N_2(g) + 3H_2(g) \rightarrow 2NH_3(g)$

b) $n_{NH_3} = 1.34 \text{ mol N}_2 \times \dfrac{2\ mol\ NH_3}{1 \text{ mol N}_2} = 2.68 \text{ mol } NH_3$

c) $m_{H_2} = \dfrac{2.75\times 10^3 \text{ g } NH_3}{17.03 \text{ g/mol}} \times \dfrac{3\ mol\ H_2}{2 \text{ mol NH}_3} \times 2.016 \text{ g/mol} = 488 \text{ g}$

d) $n_{NH_3} = \dfrac{2.92 \text{ g H}_2}{2.016 \text{ g/mol}} \times \dfrac{2 \text{ mol NH}_3}{3\ mol\ H_2} = 0.967 \text{ mol}$

$\text{NH}_3 \text{ molecules} = 0.967 \times 6.022 \times 10^{23} = 5.82 \times 10^{23} \text{ molecules}$

e) $m_{N_2} = 15.0 \text{ L} \times 79\% \times 1.25 \text{ g/L} = 14.8 \text{ g}$

$m_{NH_3} = \dfrac{14.8 \text{ g } N_2}{28.02 \text{ g/mol}} \times \dfrac{2 \text{ mol NH}_3}{1 \text{ mol N}_2} \times 17.03 \text{ g/mol} = 18.1 \text{ g}$

§ Limiting Reactant and Theoretical Yield

$2Sb(s)$	+	$3I_2(s)$	$\rightarrow$	$2SbI_3(s)$
121.8×2		$3 \times (126.9 \times 2)$		$2 \times (121.8 + 126.9 \times 3)$
$= 243.6g$		$= 763.4g$		$= 1005.0g$

└→ theoretical yield 理論產量

Limiting reactant：the reactant that produces the smaller amount is the limiting reactant.

若　3 mole Sb　3 mole I_2 $\rightarrow$ 2 SbI_3

limiting reactant　2mole

限制反應物

∴ Sb 餘 3 – 2 = 1 mole ------excess reactant

產物有： 2 mole SbI_3 及剩餘 1mole Sb

That in deciding on the theoretical yield of product, you choose the smaller of the two calculated amounts.

Ex 3.10: Determine the limiting reactant and the theoretical yield ？

$$2Sb(s) + 3I_2(s) \rightarrow 2SbI_3(s)$$

a) 1.20 mole of Sb and 2.40 mole of I_2 are mixed

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

Ans:

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

n_{SbI_3} $from$ I_2 = 2.40 mol $I_2 \times \frac{2 \text{ mol SbI}_3}{3 \text{ } mol \text{ I}_2}$ = 1.60 mol

∴ Sb is the limiting reactant; theoretical yield = 1.20 mol SbI_3.

b) m_{SbI_3} $from$ Sb = $\frac{1.20 \text{ g Sb}}{121.8 \text{ g/mol}} \times \frac{2 \text{ mol SbI}_3}{2 \text{ } mol \text{ Sb}} \times$ 502.5 g/mol = 4.95 g

m_{SbI_3} $from$ I_2 = $\frac{2.40 \text{ g I}_2}{253.8 \text{ g/mol}} \times \frac{2 \text{ mol SbI}_3}{3 \text{ } mol \text{ I}_2} \times$ 502.5 g/mol = 3.17 g (smaller)

∴ I_2 is the limiting reactant; theoretical yield = 3.17 g SbI_3.

m_{Sb} required = $\frac{3.17 \text{ g SbI}_3}{502.5 \text{ g/mol}} \times \frac{2 \text{ mol Sb}}{2 \text{ } mol \text{ SbI}_3} \times$ 121.8 g/mol = 0.768 g

m_{Sb} left = 1.20 - 0.768 = 0.43 g

Check:

$2Sb(s)$	+	$3I_2(s)$	$\rightarrow$	$2SbI_3(s)$	+	$Sb(s)$
1.20 g		2.40 g		3.17 g		0.43 g
左： 3.60 g				右：3.60 g		ok

§ Experimental yield; Percent yield

實驗　　產量　　產量百分比; 產率

Experimental yield < Theoretical yield

$$\text{Percent yield (\%)} = \frac{experimental}{theoretical} \times 100 \quad (\%)$$

Ex 3.11: Consider again the reaction discussed in Ex 3-10:

$$2Sb(s) + 3I_2(s) \rightarrow 2SbI_3(s)$$

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

Ans:

m_{SbI_3} = 1.20 mol × 502.5 g/mol = 603 g

experimental yield of SbI_3 = 603 × 78.2 % = 472 g =

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