Chapter 3: Formulae, Equations and Moles (Ch3 Chang, Ch3 Jespersen)

Mass Relationships in Chemical Reactions

Atomic mass (or weight) is the mass of an atom in *atomic mass units*.

Molecular weight is the mass of the molecule in *atomic mass units*.

The atomic mass unit, (amu) is defined as exactly $\frac{1}{12}$ of the mass of one ^{12}C atom.

1 amu = 1.66054×10^{-24} g and 1 g = 6.02214×10^{23} amu

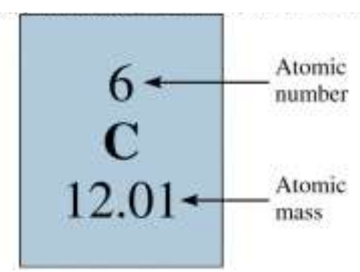
^{1}H atom = 1.6735×10^{-24} g which is 1.0078 amu.

Average Atomic Masses

The *average* atomic mass is determined by using masses of the various isotopes, and their *relative abundances*.

Carbon is 98.892% ^{12}C and 1.108% ^{13}C
^{12}C is 12 amu (exactly)
^{13}C is 13.00335 amu

(0.98892)(12 amu) + (0.01108)(13.00335 amu) = 12.011 amu



The *average atomic mass* of each element (expressed in amu) is also known as its atomic weight.

Problem: Boron obtained from borax ($Na_2B_4O_7 \cdot 10H_2O$; sodium tetraborate decahydrate) deposits in Death Valley consists of two isotopes.

They are boron-10 and boron-11 with atomic masses of 10.013 amu and 11.009 amu, respectively.

The atomic mass of boron is 10.81 amu (*see periodic table*).

What are the relative abundances of each Boron isotope in this compound ?

There are only two isotopes so

$$\begin{aligned}
10.013\,(X) + 11.009(1-X) &= 10.81 \\
10.013X + 11.009 - 11.009X &= 10.81 \\
(10.013 - 11.009)X + 11.009 &= 10.81 \\
-0.996X &= -0.199 \\
X &= \frac{-0.199}{-0.996} \\
X &= 0.19998.
\end{aligned}$$

So the relative abundances are 0.20 (20%; ^{10}B) and 0.80 (80%; ^{11}B).

The Mole and Molar Mass

The mole (mol) is defined as the amount of matter that contains as many *objects* (atom, molecules, or whatever objects we are considering) as the *number of atoms* in exactly 12 g of ^{12}C.

That number is **6.022 140 857(74) x 10^{23} mol^{-1}**.

This number is given a special name: Avogadro's number, (N_A).

Usually we will use **6.022 x 10^{23}**.

The mass of single atom of an element (in amu) is numerically equal to the mass (in grams) of 1mol of atoms of that element.

One ^{12}C atom weights 12 amu → 1 mol of ^{12}C weighs 12 g.

One ^{24}Mg atom weights 24 amu → 1 mol of ^{24}Mg weighs 24 g.

One ^{197}Au atom weights 197 amu → 1 mol of ^{197}Au weighs 197 g.

The *mass* in *grams* of 1 *mol* of a substance is called its molar mass.

Formula and Molecular Weights (Masses)

The formula weight of a substance is the *sum* of the atomic weights of *each* atom in its chemical formula.

E.g. H_2SO_4 has a formula weight of 98.09 amu.

Because FW = 2(AW of H) + (AW of S) + 4(AW of O)

= 2(1.008amu) + 32.07 + 4(16.00)

= 98.09 amu

If the chemical formula **is** the molecular formula, then the formula weight is also called the molecular weight.

E.g. glucose, $C_6H_{12}O_6$, has a molecular weight of 180.16 amu

Because MW = 6(12.01) + 12(1.008) + 6(16.00) = 180.16 amu

With ionic substances such as NaCl, it is inappropriate to speak of *molecules*. We will use the formula weight.

$$\text{FW of NaCl} \quad = \quad 22.99 + 35.45 \quad = \quad 58.44 \text{ amu}$$

The molar mass (in *grams*) of any substance is always numerically equal to its formula weight (in *amu*).

The molecular mass (also the *molecular weight*, *MW*) is the sum of all the atoms in a molecule.

The formula mass is the sum of all the atoms in the formula unit of any compound (molecular or ionic).

One H_2O molecule weighs 18.02 amu → 1 mol of H_2O weighs 18.02g.

One NO_3^- ion weighs 62.01 amu → 1 mol of NO_3^- weighs 62.01 g.

One NaCl unit weighs 58.44 amu → 1 mol of NaCl weighs 58.44 g.

Percent Composition and Empirical Formulas

Percentage Composition from Formulas

Percent composition is the *percentage* by *mass* contributed by each element in the substance.

E.g. $C_6H_{12}O_6$

MW = 180.16 amu	since	C:	6(12.01)	=	72.06
		H:	12(1.008)	=	12.096
		O:	6(16.00)	=	96.00

$$\%C = \frac{72.06}{180.16} \times 100\% = 40.00\%$$

$$\%H = \frac{12.096}{180.16} \times 100\% = 6.714\%$$

$$\%O = \frac{96.00}{180.16} \times 100\% = 53.29\%$$

Determining Empirical Formulas: Elemental analysis

The empirical formula is the smallest whole number ratio of the elements present.

It is *consistent* with the molecular formula, but does not have to be equal to it.

E.g. hydrogen peroxide, H_2O_2, MF = H_2O_2 but EF = HO.

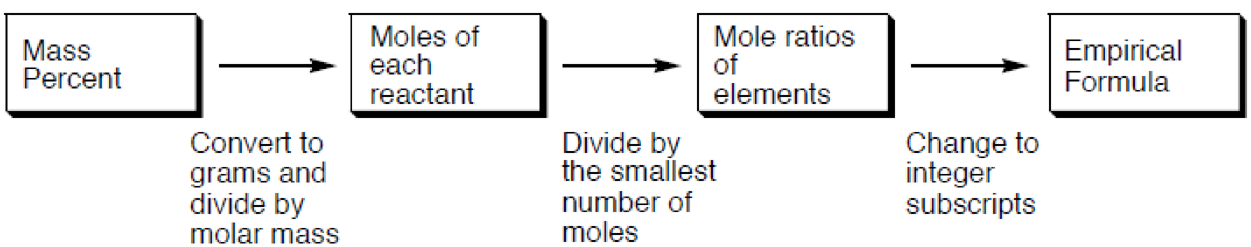
The EF is obtained from *experimental analysis* of the compound.

Analysis gives the amount of each element as a percentage. If we assume the sample to be 100 g, we can divide these masses (the percentages in grams) by the appropriate atomic weight to obtain the number of *moles* of each element in 100 g.

We then divide the larger mole numbers by the smallest mole number gives a mole ratio.

To obtain the empirical formula, change the *subscripts* to *integers*.

(The ratios may not be exact due to experimental errors).



Problem: Vitamin C (ascorbic acid) contains 40.92% C, 4.58% H, and 54.50% O by mass.

What is the empirical formula of ascorbic acid?

$$40.92 \text{ g C} \times \frac{1 \text{ mol C}}{12.01 \text{ g C}} = 3.407 \text{ mol C} \quad \frac{3.407 \text{ mol C}}{3.406} = 1 \text{ C} \xrightarrow{x3} = 3 \text{ C}$$

$$5.58 \text{ g H} \times \frac{1 \text{ mol H}}{1.008 \text{ g H}} = 4.54 \text{ mol H} \quad \frac{4.54 \text{ mol H}}{3.406} = 1.33\text{H} \xrightarrow{x3} = 4 \text{ H}$$

$$54.50 \text{ g O} \times \frac{1 \text{ mol O}}{16.00 \text{ g O}} = \boxed{3.406} \text{ mol O} \quad \frac{3.406 \text{ mol O}}{3.406} = 1 \text{ O} \xrightarrow{x3} = 3 \text{ O}$$

$$\Downarrow$$

EF = $C_3H_4O_3$

(Calculate moles of each element, then divide by the smallest mole number (3.406), and convert to smallest whole number integers, and use subscripts for the Empirical Formula).

Determination of Molecular Formulas

Molecular formula is the *actual* number of each atom in the molecule.

To calculate the molecular formula we must know the approximate molar mass.

The molar mass (of the molecule) must be an *integral multiple* of the molar mass of the empirical formula.

Problem: ascorbic acid has a molar mass of 176.12 g/mol. What is the molecular formula?

We know EF (previous slide) = $C_3H_4O_3$ = 3(12.01) + 4(1.008) + 3(16.00) = 88.06 g/mol

$$\frac{176.12 \text{ g/mol}}{88.06 \text{ g/mol}} = 2$$

So the MF = 2 x ($C_3H_4O_3$)

= $\mathbf{C_6H_8O_6}$

Empirical Formula from Combustion Analysis

<u>Problem:</u> When a 0.860 g sample of an organic compound containing C, H, and O was burned completely in oxygen, 1.64 g of CO_2 and 1.01 g of H_2O were produced.

What is the empirical formula of the compound ?

Assume all the Carbon becomes CO_2, and all the Hydrogen becomes H_2O.

Since we only have C, H and O, the Oxygen is obtained by the difference.

This much CO_2 is this number of moles

Which came from this moles of C

Which is this number of g

$$1.64 \text{ g } CO_2 \times \frac{1 \text{ mol } CO_2}{44.01 \text{ g } CO_2} \times \frac{1 \text{ mol C}}{1 \text{ mol } CO_2} \times \frac{12.01 \text{ g C}}{1 \text{ mol C}} = 0.4475 \text{ g C}$$

MW of CO_2 is 44.01 g/mol

$$1.01 \text{ g } H_2O \times \frac{1 \text{ mol } H_2O}{18.02 \text{ g } H_2O} \times \frac{2 \text{ mol H}}{1 \text{ mol } H_2O} \times \frac{1.008 \text{ g H}}{1 \text{ mol H}} = 0.1121 \text{ g H}$$

MW of H_2O is 18.02 g/mol

Mass of O = 0.860g total - (0.4475g C + 0.1121 g H)

= 0.300 g O

Now we know masses of C, H and O, we can calculate the EF like previously…

$$0.448 \text{ g C} \times \frac{1 \text{ mol C}}{12.01 \text{ g C}} = 0.0373 \text{ mol C} \qquad \frac{0.0373 \text{ mol C}}{0.0188} = 2 \text{ C}$$

$$0.112 \text{ g H} \times \frac{1 \text{ mol H}}{1.008 \text{ g H}} = 0.111 \text{ mol H} \qquad \frac{0.111 \text{ mol H}}{0.0188} = 6 \text{ H}$$

$$0.300 \text{ g O} \times \frac{1 \text{ mol O}}{16.00 \text{ g O}} = \boxed{0.0188} \text{ mol O} \qquad \frac{0.0188 \text{ mol O}}{0.0188} = 1 \text{ O}$$

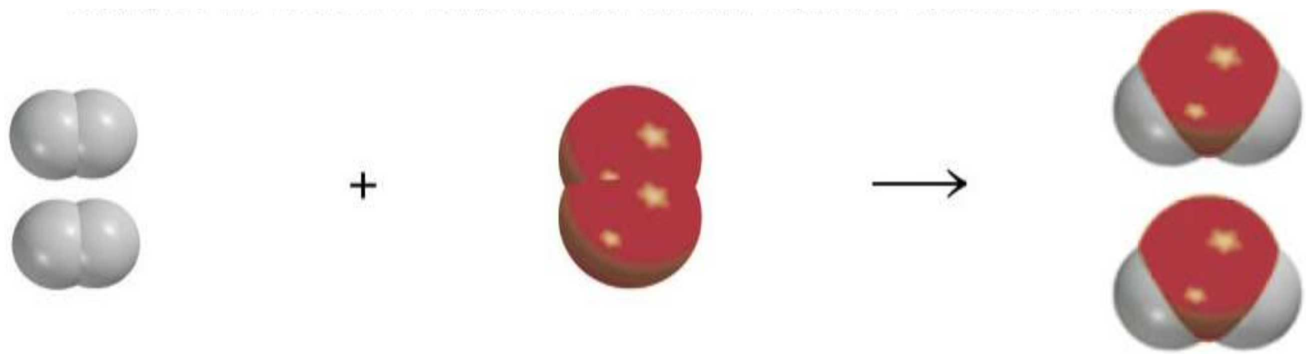
EF = C_2H_6O

Chemical Equations

A chemical reaction is defined as a process in which a substance (or substances) is changed into one or more *new substances*.

A chemical reaction is represented by a chemical equation:

E.g. $2\ H_2 \quad + \quad O_2 \quad \rightarrow \quad 2\ H_2O$



Two hydrogen molecules + One oxygen molecule ⟶ Two water molecules

On the left of the arrow:	reactants
On the right of the arrow:	products
The + means	"*reacts with*"
The → means	"*to produce*"
The coefficients indicate	*relative* amounts of substance

Equations must be balanced, which means *equal* amounts of *each* element on *each* side of the equation.

$2\,H_2 + O_2 \rightarrow 2\,H_2O$

On the left: 4 H and 2 O

On the right: 4 H and 2 O (All atoms are balanced).

When balancing an equation, never change the subscripts (as this alters the chemical identity).

Balance an equation by changing the coefficients (this only changes *relative* amounts of a substance, not the identity.

$CH_4 + O_2 \rightarrow CO_2 + H_2O$ (*unbalanced* equation:

1 C, **4** H and **2** O → 1 C, **2** H and **3** O)

$CH_4 + 2\,O_2 \rightarrow CO_2 + 2\,H_2O$ (*balanced* equation:

1 C, 4 H and 4 O → 1 C, 4 H and 4 O)

Guidelines

1. write an unbalanced equation
2. use (whole number) coefficients to indicate how many formula units are required to balance the equation
3. balance those species that occur in the *fewest* formulas on each side.
4. reduce coefficients to *smallest whole number* values
5. when balancing reactions involving organic compounds, balance in the order: C, H, O.

E.g. $KClO_3 \rightarrow KCl + O_2$ (unbalanced in O's)

$KClO_3 \rightarrow KCl + \frac{3}{2} O_2$ (balanced, but not whole numbers, so everything x2)

$\mathbf{2\ KClO_3 \rightarrow 2\ KCl + 3\ O_2}$ (balanced in K, Cl and O's)

An organic example to highlight Guideline 5

	$C_6H_{12} + O_2 \rightarrow CO_2 + H_2O$	(unbalanced in C, H and O's)
Balance C's	$C_6H_{12} + O_2 \rightarrow 6\ CO_2 + H_2O$	(unbalanced in H and O's)
Balance H's	$C_6H_{12} + O_2 \rightarrow 6\ CO_2 + 6\ H_2O$	(unbalanced in O's)
Balance O's	$C_6H_{12} + 9\ O_2 \rightarrow 6\ CO_2 + 6\ H_2O$	(balanced)

To provide additional information, chemists often indicate the physical states (phases) of the reactants and products by using the letters **g**, **l**, and **s** to denote *gas*, *liquid*, and *solid*, respectively.

Sometimes we will write (**aq**) to denote an aqueous (*water*) environment.

Chemical symbols represent both the microscopic and macroscopic level.

$2\ H_{2(g)}$	+	$O_{2(g)}$	→	$2\ H_2O_{(g)}$
2 molecules	+	1 molecule	→	2 molecules
$2(6\ \text{x}10^{23}$ molecules)	+	$6\ \text{x}10^{23}$ molecules	→	$2(6\ \text{x}10^{23}$ molecules)
2 moles	+	1 mole	→	2 moles
2 (2.02 g)	+	32.00 g	→	2 (18.02 g)
	= 36.04 g reactants		→	36.04 g products

The coefficients in a balanced chemical equation can be interpreted as both:

- the relative numbers of molecules (or formula units) involved in the reaction, and

- the relative numbers of moles.

Stoichiometry (essentially *Chemical Arithmetic*)

The term stoichiometry was first used by Richter in 1792.

It is defined as the *quantitative study of relative quantities of reactants and products in chemical reactions*.

The term is derived from the Greek words for "*element*" and "*measure*".

So for a generic balanced equation:

$$a\,A \quad + \quad b\,B \quad \rightarrow \quad c\,C \quad + \quad d\,D$$

Use **coefficients** in the balanced equation to find mole ratios

Grams of A $\Longrightarrow$ Moles of A $\Longrightarrow$ Moles of B $\Longrightarrow$ Grams of B (*and so on...*)

Use **molar mass** of A as the conversion factor

Use **molar mass** of B as the conversion factor

E.g. $2\,H_2 + O_2 \rightarrow 2\,H_2O$

$2\text{ mol }H_2 + 1\text{ mol }O_2 \rightarrow 2\text{ mol }H_2O$

Both sides of the arrow are stoichiometrically equivalent (for a *balanced* equation).

<u>Problem:</u> how many grams of H_2O can be produced from 40.0 g O_2?

$$\underbrace{40.0\text{ g }O_2 \times \frac{1\text{ mol }O_2}{32.00\text{ g }O_2}}_{\text{Moles of }O_2} \times \overbrace{\frac{2\text{ mol }H_2O}{1\text{ mol }O_2}}^{\text{Moles of }H_2O} \times \underbrace{\frac{18.02\text{ g }H_2O}{1\text{ mol }H_2O}}_{\text{Mass of }H_2O} = 45.1\text{ g }H_2O$$

Problem: For the combustion of butane, C_4H_{10}, if we burn 1.00 g of butane, what mass of CO_2 is produced ?

First we need a balanced equation:

C_4H_{10}	+	O_2	$\rightarrow$	CO_2	+	H_2O		(unbalanced)
C_4H_{10}	+	O_2	$\rightarrow$	$4\ CO_2$	+	H_2O		(balanced C)
C_4H_{10}	+	O_2	$\rightarrow$	$4\ CO_2$	+	$5\ H_2O$		(balanced C, H)
C_4H_{10}	+	$6\frac{1}{2}\ O_2$	$\rightarrow$	$4\ CO_2$	+	$5\ H_2O$		(balanced C, H, O – but not integers)
$2\ C_4H_{10}$	**+**	**$13\ O_2$**	$\rightarrow$	**$8\ CO_2$**	**+**	**$10\ H_2O$**		**(balanced)**

$$\underbrace{1.00\text{ g } C_4H_{10} \times \frac{1\text{ mol } C_4H_{10}}{58.12\text{ g } C_4H_{10}}}_{\text{Moles of } C_4H_{10}} \times \overbrace{\frac{8\text{ mol } CO_2}{2\text{ mol } C_4H_{10}}}^{\text{Moles of } CO_2} \times \underbrace{\frac{44.01\text{ g } CO_2}{1\text{ mol } CO_2}}_{\text{Mass of } CO_2} = 3.03\text{ g } CO_2$$

MW C_4H_{10} = 4 (12.01) + 10 (1.008)

= 58.12 g/mol

MW CO_2 = 44.01 g/mol

Yields of Chemical Reactions

The quantity of product that is *calculated* to form when all of the limiting reactant reacts is called the theoretical yield.

The amount *actually* obtained in a reaction is called the actual yield.

The actual yield is typically *lower* due to real practical issues such as product sticking to glassware/filter paper; evaporation; formation of byproducts; etc.

The percent yield of a reaction relates the actual yield to the theoretical (calculated) yield:

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

Reactions with Limiting Amounts of Reactants

The reagent that is completely consumed in a reaction is called the limiting reactant or limiting reagent, because it determines (*limits*) the amount of product formed.

The other reactants are sometimes called excess reactants or excess reagents.

Problem: If 5.88 g of B_2S_3 is mixed with 7.85 g of water, and the products are boric acid and hydrogen sulfide:

- Which reactant is limiting and which reactant is in excess ?
- How many grams of the excess reactant are consumed ?
- How many grams of boric acid are produced ?

$B_2S_3 + H_2O \rightarrow H_3BO_3 + H_2S$ (Got pdts in the eqn, but unbalanced)

$B_2S_3 + H_2O \rightarrow \mathbf{2}\ H_3BO_3 + H_2S$ (Now balanced in B)

$B_2S_3 + H_2O \rightarrow 2\ H_3BO_3 + \mathbf{3}\ H_2S$ (Now balanced in B and S)

$\mathbf{B_2S_3 + 6\ H_2O \rightarrow 2\ H_3BO_3 + 3\ H_2S}$ **(Balanced in B, S and O, and H)**

Now that we have a balanced equation, and know the amount of H_2O and B_2S_3, we can look at the stoichiometry…

$$\mathbf{B_2S_3 + 6\ H_2O \rightarrow 2\ H_3BO_3 + 3\ H_2S}$$

$$\underbrace{5.88 \text{ g } B_2S_3 \times \frac{1 \text{ mol } B_2S_3}{117.83 \text{ g } B_2S_3}}_{\text{Moles of } B_2S_3} \times \overbrace{\frac{2 \text{ mol } H_3BO_3}{1 \text{ mol } B_2S_3}}^{\text{Moles of } H_3BO_3} = 0.0998 \text{ mol } H_3BO_3$$

Maximum possible amount produced by this much B_2S_3

MW $B_2S_3 = 2\ (10.81) + 3\ (32.06) = 117.83$ g/mol

$$\underbrace{7.85 \text{ g } H_2O \times \frac{1 \text{ mol } H_2O}{18.02 \text{ g } H_2O}}_{\text{Moles of } H_2O} \times \overbrace{\frac{2 \text{ mol } H_3BO_3}{6 \text{ mol } H_2O}}^{\text{Moles of } H_3BO_3} = 0.145 \text{ mol } H_3BO_3$$

Maximum possible amount produced by this much H_2O

MW $H_2O = 18.02$ g/mol

B_2S_3 is the limiting reagent. (H_2O is in excess).

(All the B_2S_3 will be consumed before the H_2O. There is not enough B_2S_3 to have all the H_2O react).

- *How many grams of the excess reactant are consumed ?*

$$\underbrace{5.88 \text{ g } B_2S_3 \times \frac{1 \text{ mol } B_2S_3}{117.83 \text{ g } B_2S_3}}_{\text{Moles of } B_2S_3} \times \frac{\overbrace{6 \text{ mol } H_2O}^{\text{Moles of } H_2O}}{1 \text{ mol } B_2S_3} \times \underbrace{\frac{18.02 \text{ g } H_2O}{1 \text{ mol } H_2O}}_{\text{Mass of } H_2O} = 5.40 \text{ g } H_2O \text{ consumed}$$

5.40 g consumed from an original amount of 7.85 g, leaves (7.85 – 5.40 g) = 2.45 g of water remaining.

- *How many grams of boric acid are produced ?*

Mass of H_3BO_3

$$\underbrace{0.0998 \text{ mol } H_3BO_3}_{\text{Yield from limiting reagent}} \times \frac{61.83 \text{ g } H_3BO_3}{1 \text{ mol } H_3BO_3} = 6.17 \text{ g of } H_3BO_3 \text{ produced.}$$

MW H_3BO_3 = 61.83 g/mol

Problem: Adipic acid ($C_6H_{10}O_4$) is used to produce nylon. The acid is made commercially by controlled reaction between cyclohexane (C_6H_{12}) and O_2.

$$2\ C_6H_{12} \quad + \quad 5\ O_2 \quad \rightarrow \quad 2\ C_6H_{10}O_4 \quad + \quad 2\ H_2O \qquad \text{(balanced)}$$

Assume you carry out this reaction starting with 25.0 g of cyclohexane and that cyclohexane is the limiting reagent.

- What is the theoretical yield of adipic acid?

- If you obtain 35.5 g of adipic acid from your reaction, what is the percent yield of adipic acid ?

$$\underbrace{25.0\ \text{g}\ C_6H_{12} \times \frac{1\ \text{mol}\ C_6H_{12}}{84.16\ \text{g}\ C_6H_{12}}}_{\text{Moles of } C_6H_{12}} \times \overbrace{\frac{2\ \text{mol}\ C_6H_{10}O_4}{2\ \text{mol}\ C_6H_{12}}}^{\text{Moles of } C_6H_{10}O_4} \times \underbrace{\frac{146.14\ \text{g}\ C_6H_{10}O_4}{1\ \text{mol}\ C_6H_{10}O_4}}_{\text{Mass of } C_6H_{10}O_4} = 43.4\ \text{g of}\ C_6H_{10}O_4$$

MW C_6H_{12} = 84.16 g/mol

MW $C_6H_{10}O_4$ = 146.14 g/mol

Theoretical yield is 43.4 g.

- *If you actually obtain 35.5 g of adipic acid from your reaction, what is the percent yield of adipic acid ?*

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

$$\frac{35.5 \text{ g}}{43.4 \text{ g}} \times 100\ \% = 81.8\ \%\ \text{yield}$$

Stoichiometry Summary