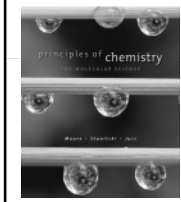

BROOKS/COLE CENGAGE Learning

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Chapter 4
Quantities of Reactants and Products

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Chemical Equations

Reactants ⟶ **Products**

$C_6H_{12}O_6(aq) \xrightarrow{\text{yeast}} 2\ C_2H_5OH(\ell) + 2\ CO_2(g)$

glucose ⟶ ethanol, carbon dioxide

Conditions may be shown over the arrow. e.g.

heat (Δ)	reflux	catalyst present (yeast)

Physical states are often listed:

(g)	gas	(s)	solid
(ℓ)	liquid	(aq)	aqueous (dissolved in water)

Chemical Equations

Balanced equations obey the law of conservation of mass (Lavoisier 1789).

"Mass is neither created nor destroyed in a chemical reaction."

$$2\ C_2H_6(g) + 7\ O_2(g) \longrightarrow 4\ CO_2(g) + 6\ H_2O(\ell)$$

	$2\ C_2H_6(g)$	$7\ O_2(g)$	$4\ CO_2(g)$	$6\ H_2O(\ell)$
Nanoscale	2 molecules	7 molecules	4 molecules	6 molecules
Macroscale	2 moles	7 moles	4 moles	6 moles
	2(30.0)= 60.0 g	7(32.0)= 224.0 g	4(44.0)= 176.0 g	6(18.0)= 108.0 g
	284.0 g		284.0 g	

C_2H_6 molar mass

O_2 molar mass

Chemical Equations

Stoichiometry

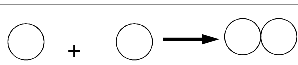
The relationship between the number of reactant and product molecules in a chemical equation.

$CaCO_3(s) + 2\ HNO_3(aq) \longrightarrow$

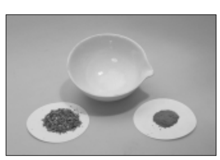
$Ca(NO_3)_2(aq) + CO_2(g) + H_2O(\ell)$

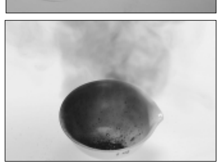
A stoichiometric coefficient

Combination Reactions



X Z XZ





Element plus halogen or O_2:

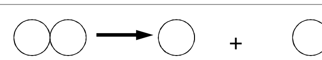
$2\ Mg(s) + O_2(g) \rightarrow 2\ MgO(s)$

$I_2(s) + Zn(s) \rightarrow ZnI_2(s)$

There are other types:

$2\ SO_2(g) + O_2(g) \rightarrow 2\ SO_3(g)$

Decomposition Reactions



XZ X Z

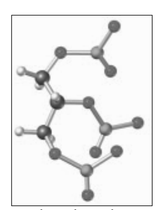
Often initiated by heat:

$CaCO_3(s) \xrightarrow{800 - 1000^\circ C} CaO(s) + CO_2(g)$

$2\ KNO_3(s) \xrightarrow{\text{heat}} 2\ KNO_2(s) + O_2(g)$

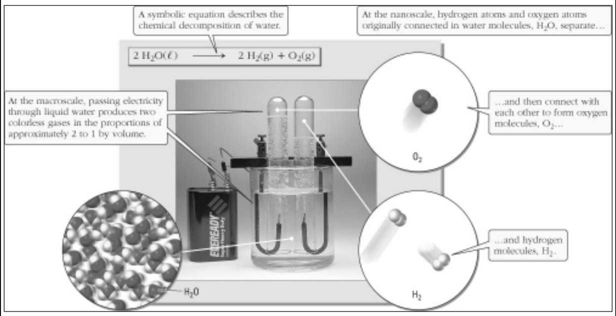
Occasionally by shock:

$4\ C_3H_5(NO_3)_3(\ell) \longrightarrow$
$12\ CO_2(g) + 10\ H_2O(\ell) + 6\ N_2(g) + O_2(g)$

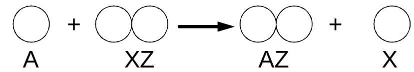


nitroglycerin

Decomposition Reactions



Displacement Reactions



Metals *may* displace another metal from its salt

$Fe(s) + CuSO_4(aq) \rightarrow FeSO_4(aq) + Cu(s)$

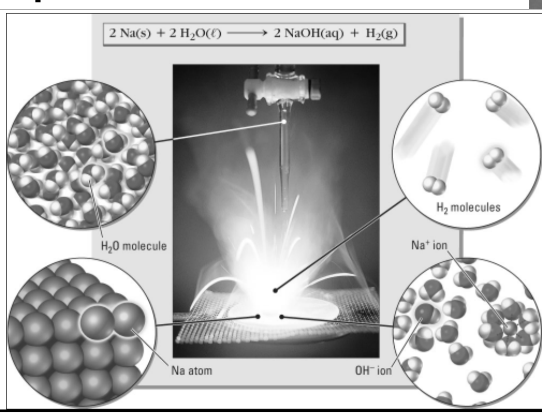
$Zn(s) + 2\ AgNO_3(aq) \rightarrow Zn(NO_3)_2(aq) + 2\ Ag(s)$

Some other examples:

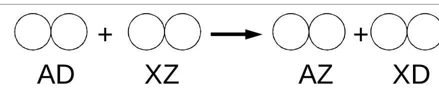
$F_2(g) + 2\ LiCl(s) \rightarrow 2\ LiF(s) + Cl_2(g)$

$2\ Na(s) + 2\ H_2O(\ell) \rightarrow 2\ NaOH(aq) + H_2(g)$

Displacement Reactions



Exchange Reactions



$AgNO_3(aq) + HCl(aq) \rightarrow AgCl(s) + HNO_3(aq)$

$Pb(NO_3)_2(aq) + K_2CrO_4(aq)$
$\rightarrow PbCrO_4(s) + 2\ KNO_3(aq)$

Balancing Chemical Equations

1. Write an unbalanced equation with correct formulas for all substances.
2. Balance the atoms of one of the elements.
   - Start with the most complex molecule.
   - Change the coefficients in front of the molecules.
   - Do NOT alter the chemical formulas.
3. Balance the remaining elements.

Balancing Chemical Equations

Balance : $Al + Fe_2O_3 \longrightarrow Al_2O_3 + Fe$

step 1 $Al + Fe_2O_3 \longrightarrow Al_2O_3 + Fe$

1 Al (2Fe + 3O) (2Al + 3O) 1Fe

not balanced / not balanced

step 2 $Al + Fe_2O_3 \longrightarrow Al_2O_3 + 2\ Fe$

1 Al (2Fe + 3O) (2Al + 3O) 2Fe

balanced / not balanced

step 3 $2\ Al + Fe_2O_3 \longrightarrow Al_2O_3 + 2\ Fe$

2Al (2Fe + 3O) (2Al + 3O) 2Fe

step 4 – balanced

Balancing Chemical Equations

Combustion of rocket fuel:

$C_2H_8N_2 + N_2O_4 \longrightarrow N_2 + H_2O + CO_2$

2C + 8H + 4N + 4O   1C + 2H + 2N + 3O

not balanced

Balance C and N in $C_2H_8N_2$ first:

$C_2H_8N_2 + N_2O_4 \longrightarrow N_2 + 4\,H_2O + 2\,CO_2$

2C + 8H + 4N + 4O   2C + 8H + 2N + 8O

Still not balanced. Adjust N and O

$C_2H_8N_2 + 2\,N_2O_4 \longrightarrow 3\,N_2 + 4\,H_2O + 2\,CO_2$

Balanced

Balancing Chemical Equations

Polyatomic ion on both sides of an equation?

- Balance as "units".

$NaNO_3(s) + H_2SO_4(aq) \longrightarrow Na_2SO_4(aq) + HNO_3(aq)$

$Na + NO_3 + 2H + SO_4$ $2Na + SO_4 + H + NO_3$

not balanced

Balance Na in Na_2SO_4

$2\,NaNO_3(s) + H_2SO_4(aq) \longrightarrow Na_2SO_4(aq) + HNO_3(aq)$

$2Na + 2NO_3 + 2H + SO_4$ $2Na + SO_4 + H + NO_3$

not balanced

$2\,NaNO_3(s) + H_2SO_4(aq) \longrightarrow Na_2SO_4(aq) + 2\,HNO_3(aq)$

$2Na + 2NO_3 + 2H + SO_4$ $2Na + SO_4 + 2H + 2NO_3$

balanced

The Mole and Chemical Reactions

$2\,C_2H_6(g) + 7\,O_2(g) \longrightarrow 4\,CO_2(g) + 6\,H_2O(\ell)$

2 moles of C_2H_6 react with 7 moles of O_2

2 moles of C_2H_6 produce 4 moles of CO_2

2 mol $C_2H_6 \equiv$ 7 mol O_2

2 mol $C_2H_6 \equiv$ 4 mol CO_2 etc.

Mole ratios:

$\frac{2\text{ mol } C_2H_6}{7\text{ mol } O_2} = 1 \qquad \frac{7\text{ mol } O_2}{2\text{ mol } C_2H_6} = 1$

The Mole and Chemical Reactions

What mass of O_2 and Br_2 is produced by the reaction of 25.0 g of TiO_2 with excess BrF_3?

$3\,TiO_2(s) + 4\,BrF_3(\ell) \rightarrow 3\,TiF_4(s) + 2\,Br_2(\ell) + 3\,O_2(g)$

Notes:

- Check the equation is balanced!
- Stoichiometric ratios:

  $3TiO_2 \equiv 3O_2$; $3TiO_2 \equiv 2Br_2$; and many others

- *Excess* BrF_3 = enough BrF_3 to react all the TiO_2.

The Mole and Chemical Reactions

What mass of O_2 and Br_2 is produced by the reaction of 25.0g of TiO_2 with excess BrF_3? $3\,TiO_2(s) + 4\,BrF_3(\ell) \rightarrow 3\,TiF_4(s) + 2\,Br_2(\ell) + 3\,O_2(g)$

n_{TiO2} = mass TiO_2 / FM TiO_2

$= 25.0 \text{ g} \times \frac{1 \text{ mol}}{79.88 \text{ g}} = 0.3130 \text{ mol } TiO_2$

3 mol $TiO_2 \equiv$ 3 mol O_2

$0.3130 \text{ mol } TiO_2 \; \frac{3 \text{ mol } O_2}{3 \text{ mol } TiO_2} = 0.3130 \text{ mol } O_2$

The Mole and Chemical Reactions

What mass of O_2 and Br_2 is produced by the reaction of 25.0g of TiO_2 with excess BrF_3? $3\,TiO_2(s) + 4\,BrF_3(\ell) \rightarrow 3\,TiF_4(s) + 2\,Br_2(\ell) + 3\,O_2(g)$

Mass of O_2 produced $= n_{O2}$ (mol. wt. O_2)

= 0.3130 mol x 32.00 g/mol

= 10.0 g

3 $TiO_2 \equiv$ 2 Br_2

$n_{Br2} = 0.3130 \text{ mol } TiO_2 \; \frac{2Br_2}{3\,TiO_2} = 0.2087 \text{ mol } Br_2$

Mass of $Br_2 = 0.2087 \text{ mol} \; \frac{159.81 \text{ g}}{\text{mol } Br_2} = 33.4 \text{ g } Br_2$

Practice Problem 4.8

The purity of Mg can be found using the reaction…

$Mg(s) + 2\,HCl(aq) \longrightarrow MgCl_2(aq) + H_2(g)$

Calculate the % Mg in a 1.72-g sample that produced 6.46 g of $MgCl_2$ when reacted with excess HCl.

More difficult – What should you calculate?

- How much pure Mg will make 6.46 g of $MgCl_2$?
- Express as a % of the original mass.

Practice Problem 4.8

$Mg + 2\,HCl \rightarrow MgCl_2 + H_2$

FW of $MgCl_2$ = 24.31 + 2(35.45) = 95.21 g/mol

$n_{MgCl2} = 6.46\text{ g } MgCl_2 \;\dfrac{1\text{ mol}}{95.21\text{ g}} = 0.06785\text{ mol } MgCl_2$

Use mole ratio 1 mol Mg ≡ 1 mol $MgCl_2$

Mg required: $0.06785\text{ mol } MgCl_2 \;\dfrac{1\text{ Mg}}{1\text{ }MgCl_2}$

= 0.06785 mol of pure Mg

Practice Problem 4.8

$Mg + 2\,HCl \rightarrow MgCl_2 + H_2$

Calculate mass of pure Mg needed

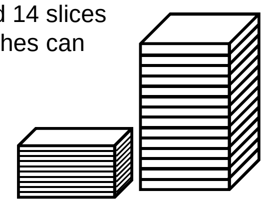
$0.06785\text{ mol Mg} \times \dfrac{24.31\text{ g}}{1\text{ mol}} = 1.649\text{ g Mg}$

Given 1.72 g of impure Mg.

Purity (as mass %) = $\dfrac{1.649\text{ g}}{1.72\text{ g}} \times 100\% = 95.9\ \%$

Reactions with Reactant in Limited Supply

Given 10 slices of cheese and 14 slices of bread. How many sandwiches can you make?



Balanced equation

1 cheese + 2 bread ⟶ 1 sandwich

1 cheese ≡ 2 bread
1 cheese ≡ 1 sandwich
2 bread ≡ 1 sandwich

Reactions with Reactant in Limited Supply

Two methods can be used:

Product Method
Calculate the product from each starting material.

- The reactant giving the smallest number is limiting.

$10\text{ cheese} \times \dfrac{1\text{ sandwich}}{1\text{ cheese}} = 10\text{ sandwiches}$

$14\text{ bread} \times \dfrac{1\text{ sandwich}}{2\text{ bread}} = 7\text{ sandwiches}$

Bread is limiting. It will be used up first

Correct answer

Reactions with Reactant in Limited Supply

Reactant Method

Pick a reactant; calculate the amount of the other(s) needed. Enough?

- Yes = Your choice is the limiting reactant.
- No = Another reactant is limiting.

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e.g. choose bread
cheese needed: 14 bread (1 cheese /2 bread) = 7
Available …. bread is limiting.

e.g. choose cheese
bread needed: 10 cheese (2 bread/1 cheese) = 20
Not available …. bread is limiting.

Reactions with Reactant in Limited Supply

Bread is limiting…

…base all other calculations on the limiting reactant.

Sandwiches made
14 bread (1 sandwich / 2 bread) = 7 sandwiches

Cheese remaining
14 bread (1 cheese / 2 bread) = 7 cheese used.
Started with 10 cheese. Cheese remaining
10 – 7 = 3 slices

Reactions with Reactant in Limited Supply

How much water will be produced by the combustion of 25.0 g of H_2 in the presence of 100. g of O_2?

Write a balanced equation:

$$2\,H_2(g) + O_2(g) \longrightarrow 2\,H_2O(\ell)$$

$$n_{H2} = 25.0\text{ g}\,\frac{1\text{ mol }H_2}{2.016\text{ g}} = 12.40\text{ mol }H_2$$

$$n_{O2} = 100.\text{ g}\,\frac{1\text{ mol }O_2}{32.00\text{ g}} = 3.125\text{ mol }O_2$$

Reactions with Reactant in Limited Supply

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

Moles: 12.40 3.125

Product Method

From H_2 $$n_{H2O} = 12.40\text{ mol }H_2\,\frac{2H_2O}{2H_2} = 12.40\text{ mol}$$

From O_2 $$n_{H2O} = 3.125\text{ mol }O_2\,\frac{2H_2O}{1O_2} = 6.250\text{ mol}$$

O_2 gave less. O_2 is limiting. Use O_2 in all calcs.

$$m_{H2O} = 6.250\text{ mol }H_2O\,\frac{18.02\text{ g}}{1\text{ mol}} = 113.\text{ g water}$$

Reactions with Reactant in Limited Supply

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

Moles available: 12.40 3.125

Reactant Method

e.g. choose H_2

O_2 needed: 12.40 mol H_2 (1 O_2 /2 H_2)= 6.20 mol

Not available …. O_2 is limiting.

You only need one calculation. Had you chosen O_2
H_2 needed: 3.125 mol O_2 (2 H_2 /1 O_2)= 6.250 mol
Available …. O_2 is limiting.

H_2O formed: 3.125 mol O_2 ($2H_2O/1O_2$) = 6.250 mol.
= 113. g

Reactions with Limited Reactants

Consider :

$$4\,NH_3(g) + 5\,O_2(g) \longrightarrow 4\,NO(g) + 6\,H_2O(g)$$

If 374 g of NH_3 and 768 g of O_2 are mixed, what mass of NO will form?

Balanced equation? yes

$$n_{NH3} = 374\text{ g}\,\frac{1\text{ mol}}{17.03\text{ g}} = 21.96\text{ mol}$$

$$n_{O2} = 768\text{g}\,\frac{1\text{ mol}}{32.00\text{ g}} = 24.00\text{ mol}$$

Reactions with Limited Reactants

$$4\,NH_3(g) + 5\,O_2(g) \longrightarrow 4\,NO(g) + 6\,H_2O(g)$$

Mol available: 21.96 24.00

From NH_3
NO formed: $$21.96\text{ mol }NH_3\,\frac{4\text{ NO}}{4\text{ }NH_3} = 21.96\text{ mol NO}$$

From O_2
NO formed: $$24.00\text{ mol }O_2\,\frac{4\text{ NO}}{5\text{ }O_2} = 19.20\text{ mol NO}$$

Smallest amount…. O_2 is limiting.

Reactions with Limited Reactants

Mass of NO formed?

$4\ NH_3(g) + 5\ O_2(g) \longrightarrow 4\ NO(g) + 6\ H_2O(g)$

~~21.96~~ mol　　24.00 mol　　　　19.20 mol

O_2 is limiting. Base all calculations on O_2.

NO formed = 19.20 mol NO

$$\text{Mass of NO} = 19.20 \text{ mol NO} \times \frac{30.01\text{g}}{1 \text{ mol}} = 576 \text{ g NO}$$

Reactions with Limited Reactants

What mass of MgI_2 is made by the reaction of 75.0 g of Mg with 75.0 g of I_2?

$Mg + I_2 \rightarrow MgI_2$

- Balanced? YES
- Calculate moles
  - 75.0 g of Mg = 75.0g/(24.31 g mol^{-1}) = 3.085 mol Mg
  - 75.0 g of I_2 = 75.0g/(253.9 g mol^{-1}) = 0.2955 mol I_2

  Limiting reactant? $1Mg \equiv 1I_2$ so I_2 = limiting
- Since $1MgI_2 \equiv 1I_2$ produce 0.2955 mol MgI_2
- Mass of MgI_2 = 0.2955 mol x 278.2 g/mol = 82.2 g

Percent Yield

Theoretical yield

The amount of product predicted by stoichiometry.

Actual yield

The quantity of desired product actually formed.

Percent yield

$$\%\text{ yield} = \frac{\text{Actual yield}}{\text{Theoretical yield}} \times 100\%$$

Percent Yield

Few reactions have 100% yield.

Possible reasons

Side reactions may produce undesired product(s).

Incomplete reaction due to poor mixing or reaching equilibrium…

Product loss during isolation and purification.

Percent Yield

2.50 g of copper heated with an excess of sulfur made 2.53 g of copper(I) sulfide

$16\ Cu(s) + S_8(s) \longrightarrow 8\ Cu_2S(s)$

What was the percent yield for this reaction?

n_{Cu} used: $2.50 \text{ g} \dfrac{1 \text{ mol}}{63.55\text{g}} = 0.03934 \text{ mol Cu}$

16 mol Cu used ≡ 8 mol Cu_2S made

Theoretical yield:

$$0.03934 \text{ mol Cu}\left(\frac{8\ Cu_2S}{16\ Cu}\right) = 0.01967 \text{ mol } Cu_2S$$

Percent Yield

2.50 g Cu + S_8 (excesss) made 2.53 g Cu_2S… What was the %-yield?

Theoretical yield = 0.01967 mol Cu_2S

$$= 0.01967 \text{ mol } Cu_2S \left(\frac{159.2 \text{ g}}{1 \text{ mol}}\right) = 3.131 \text{ g } Cu_2S$$

Actual yield = 2.53 g Cu_2S (in problem)

$$\text{Percent yield} = \frac{2.53 \text{ g}}{3.131 \text{ g}} \times 100\% = 80.8\%$$

Atom Economy

Examines the fate of all starting-material atoms.

% atom economy =

$$\frac{\text{atomic mass of atoms in useful product(s)}}{\text{atomic mass of all reactants used}} \times 100\%$$

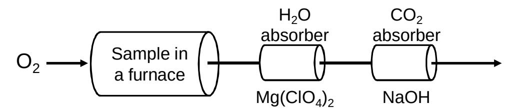
High atom economy = low waste production

Ideal reaction: high % yield and high atom economy.

Percent Composition & Empirical Formulas

Empirical formula = simplest ratio of atoms in a molecule.

Found for organic compounds by combustion analysis



C and H are converted to CO_2 & H_2O.

- Both are trapped and the weight gain measured.
- Other elements (N, O …) with other traps or by mass difference.

Percent Composition & Empirical Formulas

Vitamin C (176.12 g/mol) contains C, H & O only. If 1.000 g is burned in O2, 1.502 g CO_2 and 0.409 g H_2O form. Find its empirical & molecular formula.

Mass of C

$$1.502 \text{ g } CO_2 \; \frac{1 \text{ mol } CO_2}{44.009 \text{ g } CO_2} \; \frac{1 \text{ mol C}}{1 \text{ mol } CO_2} \; \frac{12.011 \text{ g C}}{1 \text{ mol C}} = 0.4099 \text{ g C}$$

or

$$1.502 \text{ g } CO_2 \; \frac{12.011 \text{ g C}}{44.009 \text{ g } CO_2} = 0.4099 \text{ g C}$$

Percent Composition & Empirical Formulas

Vitamin C contains C, H & O only. Combustion of 1.000 g of vitamin C produced 1.502 g of CO_2 and 0.409 g of H_2O.

Mass of H

$$0.409 \text{ g } H_2O \; \frac{2.0158 \text{ g H}}{18.015 \text{ g } H_2O} = 0.04577 \text{ g H}$$

mass of O = sample mass – (mass of C + mass of H)

Mass of O = 1.000 g – (0.4099 g + 0.04577 g)
= 0.544 g

Percent Composition & Empirical Formulas

Convert to moles:

$$\frac{0.4099 \text{ g C}}{12.011 \text{ g/mol}} = 0.03413 \text{ mol C}$$

$$\frac{0.04577 \text{ g H}}{1.0079 \text{ g/mol}} = 0.04541 \text{ mol H}$$

$$\frac{0.544 \text{ g O}}{15.999 \text{ g/mol}} = 0.0340 \text{ mol O}$$

Percent Composition & Empirical Formulas

Find the mole ratio (divide by smallest…):

C 0.03413 / 0.0340 = 1.00

H 0.04541 / 0.0340 = 1.34

O 0.0340 / 0.0340 = 1.00

Close to 1 : 1⅓ : 1 (C : H : O)

Multiply by 3 to get an integer ratio (3 : 4 : 3)

Empirical formula is $C_3H_4O_3$

Percent Composition & Empirical Formulas

…Vitamin C contains C, H & O only… … molar mass of vitamin C is 176.12 g/mol, find its empirical and molecular formula.

Empirical formula = $C_3H_4O_3$

Empirical mass = 3(12) + 4(1) + 3(16) g = 88 g

Molar mass = 176.12 g

Molar mass ≈ 2 x (empirical mass)

Vitamin C has the molecular formula $C_6H_8O_6$