Chapter 3

Chemical Equations & Reaction Stoichiometry

I) Chemical Equations

Symbolic representation of a chemical reaction

potassium + water $\longrightarrow$ potassium hydroxide + hydrogen

$$2\ K(s) + 2\ H_2O(\ell) \rightarrow 2\ KOH(aq) + H_2(g)$$

Coefficients

indicate the number of atoms, molecules or formula units of each substance involved in the rxn.

2 atoms of potassium react w.
2 molecules of water to produce
2 f.u. of potassium hydroxide &
1 molecule of hydrogen

(s) ≡ solid
(g) ≡ gas

(ℓ) ≡ liquid
(aq) ≡ aqueous soln (in H_2O)

$$KClO_4(s) \xrightarrow[Fe_2O_3]{\Delta} KCl(s) + 2\ O_2(g)$$

Δ ≡ heat

Fe_2O_3 ≡ catalyst (makes rx happen faster)

$$N_2(g) + 3\ H_2(g) \underset{Fe\ \ K_2O\ \ Al_2O_3}{\overset{550°C,\ 350\ atm}{\rightleftharpoons}} 2\ NH_3(g)$$

II) Balancing Chemical Eqn.

Law of Conservation of Mass

- mass neither created nor destroyed
  - just rearrangement of atoms

# atoms of each element in reactants	=	# atoms of each element in products

Balance atoms ⇒ balance mass

A) General Method for Balancing Equations

Requirements

1. Correct chemical formulas must be used for all reactants and products.
2. The number of atoms of each element in the reactants must equal the number of atoms of each element in the products.
3. Any charge on the left must equal any charge on the right.
4. Only the smallest whole number coefficients are acceptable.

Guidelines

1. Disregarding hydrogen, oxygen, and polyatomic ions, find the molecule containing the largest number of atoms of a single element. Balance that element first.
2. Balance polyatomic ions as a unit, if they remain unchanged.
3. Balance hydrogen and oxygen last. If either appears in elemental form, it is balanced last.
4. Check to see that all atoms are balanced and the smallest whole number coefficients are used.

B) Ex 1 : Solid potassium nitrate decomposes when heated to produce solid potassium nitrite & oxygen gas

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C) <u>Ex 2</u> : Write the balanced eqn. for the production of acetylene, C_2H_2, from calcium carbide, CaC_2, & water.

$$CaC_2(s) + H_2O(\ell) \longrightarrow Ca(OH)_2(aq) + C_2H_2(g)$$

D) Ex 3 : Write the balanced eqn. for the combustion of acetylene.

E) Ex 4 : Calcium oxide reacts w. phosphoric acid to produce calcium phosphate and water.

III) Simple Patterns of Chemical Reactivity

Classify reactions by general type and predict products

Note:

Elements in the same group tend to undergo similar reactions

A) Combination Reactions

2 or more reactants combine to give 1 product.

1) Direct combination of Elements

$$3\ H_2 + N_2 \longrightarrow 2\ NH_3$$

$$Sn + 2\ Cl_2 \longrightarrow SnCl_4$$

$$8\ Zn + S_8 \longrightarrow 8\ ZnS$$

2) Combination of Cmpd. & Element

$$C_2H_4 + H_2 \longrightarrow C_2H_6$$

$$2\ NO + O_2 \longrightarrow 2\ NO_2$$

$$PF_3 + F_2 \longrightarrow PF_5$$

3) Rx. of oxides w. water

a) Metal Oxides

Basic oxides
- produce basic metal hydroxides

$$K_2O + H_2O \longrightarrow 2\,KOH$$

$$CaO + H_2O \longrightarrow Ca(OH)_2$$

b) Nonmetal oxides

Acidic oxides
- produce acids

$$SO_3 + H_2O \longrightarrow H_2SO_4$$

$$CO_2 + H_2O \longrightarrow H_2CO_3$$

B) Decomposition Reactions

Single cmpd. breaks down into 2 or more simpler substances

$$2\ NH_3 \longrightarrow 3\ H_2 + N_2$$

$$PF_5 \longrightarrow PF_3 + F_2$$

$$CaCO_3 \longrightarrow CaO + CO_2$$

$$2\ NaHCO_3 \longrightarrow Na_2CO_3 + H_2O + CO_2$$

$$2\ KClO_3 \longrightarrow 2\ KCl + 3\ O_2$$

$$2\ KNO_3 \longrightarrow 2\ KNO_2 + O_2$$

C) Combustion

Reaction w. O_2

1) Complete Combustion

$$C_2H_5OH + 3\ O_2 \longrightarrow 2\ CO_2 + 3\ H_2O$$

$$2\ C_2H_5SH + 9\ O_2 \longrightarrow 4\ CO_2 + 6\ H_2O + 2\ SO_2$$

2) Incomplete Combustion

$$C_2H_5OH + 2\ O_2 \longrightarrow 2\ CO + 3\ H_2O$$

IV) Molecular & Formula Weights

A) Molecular Weights

Sum of the atomic weights of the atoms in the molecule

1) Ex 1: Find the M.W. of the ethyl alcohol (ethanol), C_2H_6O

B) <u>Formula Weights</u>

Used for ionic substances

- consists of formula units, *NOT* molecules

<u>Formula Wt.</u>

Sum of the atomic weights of the atoms as given in the formula

1) <u>Ex 1</u>: What is the F.W. of $(NH_4)_2CO_3$?

C) Percent Composition

$$\textbf{mass \% of an element} = \frac{\text{mass of element}}{\text{Total mass}} \times 100\%$$

1) Ex 1: Determine the mass % comp. of copper (II) nitrate.

V) Avogadro's Number & the Mole

How do you weigh out the same number of items?

If we weigh quantities in ratios of weights of individual items, we obtain equal numbers of items.

A) The Mole

A.W. of H	A.W. of C
1.008 amu	12.011 amu
1 atom of H	1 atom of C
1.008 amu	12.011 amu
10 atoms of H	10 atoms of C
10.08 amu	120.11 amu
X atoms of H	Y atoms of C
1.008 g	12.011 g

X = Y = 6.022×10^{23} atoms

Avogadro's Number, $\mathbf{N_A}$

The unit for a very large number of particles is

Mole

1 mole = 6.02×10^{23} particles

1 mole C = 6.02×10^{23} C atoms = 12.011g C

1) Molar Mass

Mass in grams numerically equal to A.W., M.W., or F.W.

a) A given AW tells you:

1) avg. mass of a single atom;
amu

2) mass of a mole of atoms;
grams / mole

2) Apply to Molecules & f.u.

1mol C_2H_6O = 6.02 x 10^{23} molecules C_2H_6O

= 46.08 g C_2H_6O

1 mol $(NH_4)_2CO_3$ = 6.02 x 10^{23} $(NH_4)_2CO_3$ f.u.

= 96.11 g $(NH_4)_2CO_3$

Note: 1 mol of $(NH_4)_2CO_3$ contains:

2 x (1 mol) NH_4^+ ions

2 x (6.02 x 10^{23}) NH_4^+ ions

8 mol H atoms

B) Calculations

1) Ex 1: How many moles of He are in 40.0 g of He?

1 mol He = 6.02 x 10^{23} He atoms = 4.00 g He

2) Ex 2: How many grams of $(NH_4)_2S$ are required to obtain 0.50 mol of NH_4^+?

a) Need FW

__ N x 14.01 amu =

__ H x 1.01 amu =

__ S x 32.06 amu = ______________

1 mol $(NH_4)_2S$ =

1 mol $(NH_4)_2S$ =

3) Ex 3: Typically smog contains about 0.040 g CO per m^3 of air. How many molecules of CO are in a m^3 of air?

MW of CO =

$$1 \text{ mol} \begin{Bmatrix} \text{atoms} \\ \text{molecules} \\ \text{f.u.} \end{Bmatrix} = \begin{Bmatrix} \text{AW (g)} \\ \text{MW (g)} \\ \text{FW (g)} \end{Bmatrix} = 6.02 \times 10^{23} \begin{Bmatrix} \text{atoms} \\ \text{molecules} \\ \text{f.u.} \end{Bmatrix}$$

VI) Empirical & Molecular Formulas

A) Molecular Formula

Actual numbers and kinds of atoms in a molecule

C_6H_6	Benzene
C_2H_5OH	Ethanol

B) Empirical Formula

Relative number of atoms of each kind in a molecule

- smallest whole-number ratio of atoms

C_1H_1 Benzene or acetylene

Subscripts in a molecular formula are always some integer multiple of subscripts in empirical formula

C) Procedure for Determining E.F.

1) Express composition in grams.

   If % comp. given,
   assume 100 g sample

2) Determine # moles of each element

3) Divide by smallest # moles to obtain mole ratio - this is also the atom ratio

4) If needed: Multiply by simplest factor to get whole numbers

5) Write the formula

6) Ex 1: A 10.45 g sample of Bi combines w. oxygen to produce 11.65 g of a bismuth oxide.

Determine the E.F. of the oxide.

a) Step 1: determine mass of oxygen

b) Step 2: Convert to moles

c) Step 3: Determine mole ratio
Divide by smallest # moles

d) Step 4: Multiply by factor to get whole numbers

Bi: O:

e) Step 5: Write formula

D) Molecular Formula Determination

Molecular formula is always some integer multiple of the E.F.

	EF	MF
Benzene	CH	C_6H_6
Acetylene	CH	C_2H_2

MF = $(CH)_n$

n = multiplying factor

$$n = \frac{MW}{EFW}$$

Find MW experimentally

Benzene	Acetylene
$n = \frac{78.1 \text{ amu}}{13.0 \text{ amu}} = 6$	$n = \frac{26.0 \text{ amu}}{13.0 \text{ amu}} = 2$

1) Ex : Analysis of an unknown cmpd. gave 39.72% C, 1.67% H, 58.61% Cl. The MW was found to be 181.4 amu. Determine the molecular formula.

a) Determine Emp. Formula

C:

H:

Cl:

C:

H:

Cl:

E.F. = C H Cl

E.F.W. =

b) <u>Determine Molecular Formula</u>

$$n = \frac{MW}{EFW} = \frac{181.4 \text{ amu}}{\quad} =$$

MF =

E) Combustion Analysis

"Burn" a cmpd. containing C, H & O and use the quantities of the products, CO_2 & H_2O, to determine the amt's. of C, H & O in original cmpd.

mass CO_2 ⇒ mass C

mass H_2O ⇒ mass H

1) Ex : An unknown cmpd. contains only C, H & O. Complete combustion of a 0.1000g sample produced:

0.1910 g CO_2 0.1172 g H_2O

a) Step 1: find mass of each element

$$? \text{ g C} = 0.1910 \text{ g } CO_2 \times \frac{12.01 \text{ g C}}{44.01 \text{ g } CO_2} = 0.05212 \text{ g C}$$

Mass fraction of C in CO_2

$$? \text{ g H} = 0.1172 \text{ g } H_2O \times \frac{2(1.008) \text{ g H}}{18.02 \text{ g } H_2O} = 0.01311 \text{ g H}$$

mass O = 0.1000 g – 0.05212 g – 0.01311 g

= 0.03477 g O

b) Step 2: find mol each element

VII) Stoichiometry & the Balanced Eqn.

Determination of quantities of reactants & products involved in chem. rx's.

Use balanced chem. eqn.

- tells you not only the reactants & products but also how much of each is involved in the chem. rx.

$2\,K(s)$ +	$2\,H_2O(\ell)$ →	$2\,KOH(aq)$ +	$H_2(g)$
2 atoms	2 molecules	2 formula units	1 molecule
2 moles	2 moles	2 moles	1 mole
2 x 39 =	2 x 18 =	2 x 56 =	1 x 2 =
78g	36g	112g	2g

A) Procedure

1) Calc. Number of moles of a given substance

$$\text{grams of given} \xrightarrow[\text{mol/g}]{\frac{1}{AW} \text{ or } \frac{1}{MW} \text{ or } \frac{1}{FW}} \text{mol of given}$$

2) Determine moles of desired subst.

- use coeff. in the bal. eqn.
- convert moles of given substance to moles of desired substance

$$\text{mol of given} \xrightarrow{\text{mole ratio}} \text{mol of desired}$$

$$\text{mole ratio} = \frac{\text{moles of desired substance}}{\text{moles of given substance}}$$

$$\text{mole ratio} = \frac{\text{coeff. of desired substance}}{\text{coeff. of given substance}}$$

3) Convert moles of desired substance to grams

$$\text{mol of desired} \xrightarrow[\text{g/mol}]{\text{AW or MW or FW}} \text{grams of desired}$$

4) Summary

$$\text{grams of given} \xrightarrow{\frac{1}{MW}} \text{moles of given} \xrightarrow{\text{mole ratio}} \text{moles of desired} \xrightarrow{MW} \text{grams of desired}$$

↑ (mole ratio)

coeff. from the Bal. eqn.

VIII) Solving Stoichiometry Problems

A) Ex 1: mole given $\longrightarrow$ mole desired

How many moles of chloroform, $CHCl_3$, would be produced by the reaction 1.3 mol of chlorine?

$$CH_4 + 3\,Cl_2 \longrightarrow CHCl_3 + 3\,HCl$$

B) Ex 2: mole → mole → grams

given desired desired

How many grams of chlorine are req. to produce 0.67 mol of $CHCl_3$?

C) Ex 3:

grams → moles → moles → grams
given given desired desired

Hydrazine reacts w. hydrogen peroxide according to the following eqn.,

$$1\ N_2H_4 + 2\ H_2O_2 \rightarrow N_2 + 4\ H_2O$$

How many grams of H_2O_2 are required to react w. 1.0×10^3 g of N_2H_4?

IX) Limiting Reactant

Limiting reactant (reagent):

Reactant which is entirely consumed when a rxn. goes to completion

- limits the amount of product formed

other reactants are called excess reactants (reagents)

A) Ex 1: For the following rx., if a rxn. mixture is prepared using 1.00 kg of each reactant, how much HCN could be produced?

$$2\ CH_4 + 3\ O_2 + 2\ NH_3 \rightarrow 2\ HCN + 6\ H_2O$$

Determine the limiting reactant:

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X) Theoretical & Percent Yields

Theorectical Yield: amt. product which can be obtained from a given amt. of reactant if ALL of it reacts completely according to the given eqn.

Actual Yield : amt. product actually obtained

- usually < theoretical yield

Percent Yield : how close actual yield is to theoretical yield

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

A) Ex 1 : If only 410 g HCN is produced in the lab from the rxn. mixture in the previous ex., what is the % yield?

$$\% \text{ yield} = \frac{\text{g HCN}}{\text{g HCN}} \times 100\ \%$$