CHAPTER 3: Stoichiometry I: Equations, the Mole, and Chemical Formulas

3.1 Chemical Equations

$C_5H_{12} + O_2 \rightarrow H_2O + CO_2$
reactants   products

Use subscripts (s), (l), (g), (aq) to indicate physical states

Balancing Chemical Equations

$Al + H_2SO_4 \rightarrow Al_2(SO_4)_3 + H_2$
$Be_2C + H_2O \rightarrow Be(OH)_2 + CH_4$
$CH_4 + Br_2 \rightarrow CBr_4 + HBr$
$Cl_2 + NaI \rightarrow NaCl + I_2$
$CO + O_2 \rightarrow CO_2$
$CO_2 + KOH \rightarrow K_2CO_3 + H_2O$
$Cu(NO_3)_2 \rightarrow CuO + NO_2 + O_2$
$Fe_2O_3 + CO \rightarrow Fe + CO_2$
$Fe_2O_3 + CO \rightarrow Fe_3O_4 + CO_2$
$H_2 + Br_2 \rightarrow HBr$
$H_2O_2 \rightarrow H_2O + O_2$
$HCl + CaCO_3 \rightarrow CaCl_2 + H_2O + CO_2$
$K + H_2O \rightarrow KOH + H_2$
$KClO_3 \rightarrow KCl + O_2$
$KClO_3 \rightarrow KClO_4 + KCl$
$KNO_3 \rightarrow KNO_2 + O_2$
$KO_2 + H_2O + CO_2 \rightarrow KHCO_3 + O_2$

$Mg + O_2 \rightarrow MgO$
$N_2 + H_2 \rightarrow NH_3$
$(NH_4)_2Cr_2O_7 \rightarrow Cr_2O_3 + H_2O + N_2$
$N_2H_4 + N_2O_4 \rightarrow N_2 + H_2O$
$NaHCO_3 \rightarrow Na_2CO_3 + H_2O + CO_2$
$NH_3 + CuO \rightarrow Cu + N_2 + H_2O$
$NH_3 + O_2 \rightarrow N_2 + H_2O$
$NH_3 + O_2 \rightarrow NO + H_2O$
$NH_4NO_2 \rightarrow N_2 + H_2O$
$NH_4NO_3 \rightarrow N_2O + H_2O$
$O_3 \rightarrow O_2$
$P_4O_{10} + H_2O \rightarrow H_3PO_4$
$PbS + O_2 \rightarrow PbO + SO_2$
$S + HNO_3 \rightarrow H_2SO_4 + NO_2 + H_2O$
$S_8 + O_2 \rightarrow SO_2$
$XeF_2 + H_2O \rightarrow Xe + HF + O_2$
$Zn + AgCl \rightarrow ZnCl_2 + Ag$

Types of Chemical Reactions

Combustion: reaction with oxygen
$C + O_2 \rightarrow CO_2$
$CH_4 + O_2 \rightarrow CO_2 + H_2O$
$Fe + O_2 \rightarrow Fe_2O_3$
$C_{12}H_{22}O_{11} + O_2 \rightarrow CO_2 + H_2O$

Neutralization: reaction of acid and base to yield water and salt
$KOH + H_3PO_4 \rightarrow K_3PO_4 + H_2O$
$NaOH + H_2SO_4 \rightarrow Na_2SO_4 + H_2O$

3.2 The Mole

Atomic Masses

Atomic masses originally defined as relative masses based on H. Changed to O to improve accuracy, and to ^{12}C (1961). Masses can be determined accurately with a mass spectrometer.

For atoms which exist as isotopes, the atomic mass given is the weighted average of the isotopoc masses.

^{12}C = 12 (by definition), 98.89%

^{13}C = 13.00335, 1.11%

To calculate weighted average, multiply each isotopic mass by its relative abundance.

$C = (12.00000)(0.9889) + (13.00335)(0.0111) = 11.86680 + 0.14434 = 12.01114$

however, relative abundance is only accurate to 4 significant figures, so the atomic mass of C is given as 12.01

^{6}Li = 6.01512, 7.42%

^{7}Li = 7.01600, 92.58%

$Li = (6.01512)(0.0742) + (7.01600)(0.9258) = 6.942$

The Mole

A mole is a way to count atoms

1 mole = large number of atoms

since atoms are too small to count, we must count them indirectly by weighing then, so we define the mole in terms of mass

1 mole = number of atoms in 12 g of ^{12}C

Because 12 is the atomic mass of ^{12}C, and the atomic mass scale is a relative scale, any time you have a mass in grams equal to the atomic mass of an element, you have one mole of the element.

1 mole = 6.02214×10^{23} atoms = atomic mass in grams

for Fe, 1 mole Fe = 6.022×10^{23} atoms Fe = 55.85 g Fe

$$10.00 \text{ g Fe} \times \frac{1 \text{ mole Fe}}{55.85 \text{ g Fe}} = 0.1791 \text{ mol Fe}$$

$$17.50 \text{ mol Fe} \times \frac{55.85 \text{ g Fe}}{1 \text{ mol Fe}} = 977.4 \text{ g Fe}$$

$$1.000 \text{ g Fe} \times \frac{6.02214 \times 10^{23} \text{ atoms Fe}}{55.85 \text{ g Fe}} = 1.078 \times 10^{22} \text{ atoms Fe}$$

Molecular Weight

molecular mass = sum of masses of all atoms in molecule

for C_2H_6, molecular mass = 2(12.01 amu) + 6(1.008 amu) = 30.07 amu

1 mol C_2H_6 = 6.022×10^{23} molecules C_2H_6 = 30.07 g C_2H_6

molar mass - mass in grams of one mole of a substance

$$10.00 \text{ g } C_2H_6 \times \frac{1 \text{ mol } C_2H_6}{30.07 \text{ g } C_2H_6} = 0.3324 \text{ mol } C_2H_6$$

$$10.00 \text{ g } C_2H_6 \times \frac{6.022 \times 10^{23} \text{ molecules } C_2H_6}{30.07 \text{ g } C_2H_6} = 2.002 \times 10^{23} \text{ molecules } C_2H_6$$

$$2.002 \times 10^{23} \text{ molecules } C_2H_6 \times \frac{6 \text{ H atoms}}{1 \text{ molecule } C_2H_6} = 1.201 \times 10^{24} \text{ H atoms}$$

3.3 Empirical Formulas

$C_2H_4O_2$	C	2(12.01) =	24.02
	H	4(1.008) =	4.032
	O	2(16.00) =	32.00
			60.05

$$\%C = \frac{24.02}{60.05} \times 100\% = 40.00\%$$

$$\%H = \frac{4.032}{60.05} \times 100\% = 6.714\%$$

$$\%O = \frac{32.00}{60.05} \times 100\% = 53.29\%$$

Determining the Formula of a Compound

$$93.70\% \text{ C} \times \frac{1 \text{ mol C}}{12.01 \text{ g C}} = 7.80 \text{ mol C}$$

$$6.30\% \text{ H} \times \frac{1 \text{ mol H}}{1.008 \text{ g H}} = 6.24 \text{ mol H}$$

reduce to a simple ratio

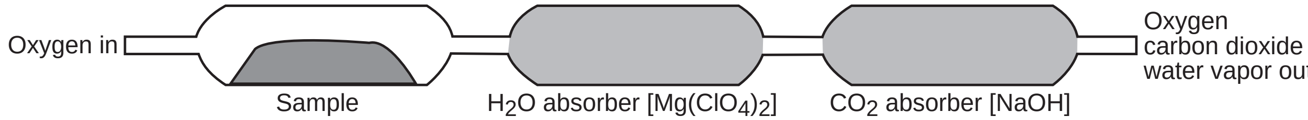
$$\frac{7.80 \text{ mol C}}{6.24 \text{ mol H}} = \frac{1.25 \text{ mol C}}{1 \text{ mol H}} = \frac{5 \text{ mol C}}{4 \text{ mol H}}$$

empirical formula is C_5H_4 empirical formula mass = 5(12.01) + 4(1.008) = 64.09

molecular mass (determined by experiment) = 128.18

$$\frac{\text{molecular mass}}{\text{formula mass}} = \frac{128.18}{64.09} = 2$$ so molecular formula = 2(empirical formula) = $C_{10}H_8$

Combustion Train



10.000 g of a compound containing C, H, and O → 21.193 g CO_2 and 3.253 g H_2O

$$21.193 \text{ g CO2 x } \frac{12.01 \text{ g C}}{44.01 \text{ g } CO_2} = 5.783 \text{ g C}$$

$$3.253 \text{ g } H_2O \text{ x } \frac{2.016 \text{ g H}}{18.016 \text{ g } H_2O} = 0.364 \text{ g H}$$

10.000 g compound - 5.783 g C - 0.364 g H = 3.853 g O

$$5.783 \text{ g C x } \frac{1 \text{ mol C}}{12.01 \text{ g C}} = 0.4815 \text{ mol C} \div 0.361 = 1.33 \text{ mol C}$$

$$0.364 \text{ g H x } \frac{1 \text{ mol H}}{1.008 \text{ g H}} = 0.361 \text{ mol H} \div 0.361 = 1.00 \text{ mol H}$$

$$3.853 \text{ g O x } \frac{1 \text{ mol O}}{16.00 \text{ g O}} = 0.2408 \text{ mol O} \div 0.361 = 0.667 \text{ mol O}$$

multiply by 3 to convert fractions → $C_4H_3O_2$ empirical formula mass = 83.06
from experiment, molecular mass = 166.13 so molecular formula = $C_8H_6O_4$

3.4 Mass Relationships in Equations

$Ca_3N_2 + 6H_2O \rightarrow 3Ca(OH)_2 + 2NH_3$

What mass of calcium hydroxide can be produced by the reaction of 100.00 g calcium nitride with excess water?

1) convert mass of calcium nitride to moles
100.00 g Ca_3N_2 x \f(148.26 g Ca_3N_2) = 0.6745 mol Ca_3N_2
2) convert moles of calcium nitride to moles of calcium hydroxide

$$0.6745 \text{ mol } Ca_3N_2 \text{ x } \frac{3 \text{ mol } Ca(OH)_2}{1 \text{ mol } Ca_3N_2} = 2.024 \text{ mol } Ca(OH)_2$$

3) convert moles of calcium hydroxide to mass of calcium hydroxide

$$2.024 \text{ mol } Ca(OH)_2 \text{ x } \frac{74.10 \text{ g } Ca(OH)_2}{1 \text{ mol } Ca(OH)_2} = 149.93 \text{ g } Ca(OH)_2$$

$H_2O + Cl_2O \rightarrow 2HOCl$

How many grams of Cl_2O are required to make 15.000 g HOCl?

$$15.000 \text{ g HOCl x } \frac{1 \text{ mol HOCl}}{52.46 \text{ g HOCl}} \text{ x } \frac{1 \text{ mol } Cl_2O}{2 \text{ mol HOCl}} \text{ x } \frac{86.90 \text{ g } Cl_2O}{1 \text{ mol } Cl_2O} = 12.42 \text{ g } Cl_2O$$

3.5 Limiting Reactants

$$Ca_3(PO_4)_2 + 8C \rightarrow Ca_3P_2 + 8CO$$

What mass of Ca_3P_2 can be produced from 50.00 g $Ca_3(PO_4)_2$ and 25.00 g C?

$$50.00\text{ g } Ca_3(PO_4)_2 \times \frac{1\text{ mol } Ca_3(PO_4)_2}{310.18\text{ g } Ca_3(PO_4)_2} = 0.1612\text{ mol } Ca_3(PO_4)_2$$

$$25.00\text{ g C} \times \frac{1\text{ mol C}}{12.01\text{ g C}} = 2.082\text{ mol C}$$

$$\frac{2.082\text{ mol C}}{0.1612\text{ mol } Ca_3(PO_4)_2} = \frac{12.9}{1} > \frac{8}{1}$$ soC is in excess and $Ca_3(PO_4)_2$ will run out first

$$0.1612\text{ mol } Ca_3(PO_4)_2 \times \frac{1\text{ mol } Ca_3P_2}{1\text{ mol } Ca_3(PO_4)_2} \times \frac{182.18\text{ g } Ca_3P_2}{1\text{ mol } Ca_3P_2} = 29.37\text{ g } Ca_3P_2$$

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

What mass of Ag can be fromed from 3.22 g Zn and 4.35 g $AgNO_3$?

$$3.22\text{ g Zn} \times \frac{1\text{ mol Zn}}{65.39\text{ g Zn}} = 0.0492\text{ mol Zn}$$

$$4.35\text{ g } AgNO_3 \times \frac{1\text{ mol } AgNO_3}{169.9\text{ g } AgNO_3} = 0.0256\text{ mol } AgNO_3$$

Zn is in excess

$$0.0256\text{ mol } AgNO_3 \times \frac{2\text{ mol Ag}}{2\text{ mol } AgNO_3} \times \frac{107.9\text{ g Ag}}{1\text{ mol Ag}} = 2.76\text{ g Ag}$$

$$4LiH + AlCl_3 \rightarrow LiAlH_4 + 3LiCl$$

What mass of $LiAlH_4$ can be formed from 40.00 g LiH and 100.00 g $AlCl_3$?

$$40.00\text{ g LiH} \times \frac{1\text{ mol LiH}}{7.949\text{ g LiH}} = 5.032\text{ mol LiH}$$

$$100.00\text{ g } AlCl_3 \times \frac{1\text{ mol } AlCl_3}{133.33\text{ g } AlCl_3} = 0.7500\text{ mol } AlCl_3$$

$$\frac{5.032\text{ mol LiH}}{0.7500\text{ mol } AlCl_3} = \frac{6.7}{1}$$ so LiH is in excess

$$0.7500\text{ mol } AlCl_3 \times \frac{1\text{ mol } LiAlH_4}{1\text{ mol } AlCl_3} \times \frac{37.95\text{ g } LiAlH_4}{1\text{ mol } LiAlH_4} = 28.46\text{ g } LiAlH_4$$

Percent Yield

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

example: if 24.04 g $LiAlH_4$ is actually obtained,

$$\%\text{ yield} = \frac{24.04\text{ g}}{28.46\text{ g}} \times 100\% = 84.5\%$$