Outline

- Chemical Calculations
- Limiting Reactant
- Heat of Reaction

Chemical Calculations

<u>Stoichiometry</u> is the study of numerical relationships in chemical reactions

Coefficients in balanced chemical equations used to generate mol-mol relationships…

$$P_4O_{10}(s) + 6H_2O(l) \rightarrow 4H_3PO_4(aq)$$

$$\frac{1\ \text{mol}\ P_4O_{10}}{4\ \text{mol}\ H_3PO_4} \quad \text{and} \quad \frac{4\ \text{mol}\ H_3PO_4}{1\ \text{mol}\ P_4O_{10}}$$

<u>Mole ratios</u> used to relate one chemical species to another in chemical calculations

Two air pollutants in car exhaust are CO and NO. These pollutants react within the car's catalytic converter to form CO_2 and N_2.

$$2CO(g) + 2NO(g) \rightarrow 2CO_2(g) + N_2(g)$$

How many mol of N_2 are produced from 3.50 mol CO?

$$3.50 \text{ mol CO} \times \frac{1 \text{ mol } N_2}{2 \text{ mol CO}} = \underline{1.75 \text{ mol } N_2}$$

How many mol of NO are needed to react with 2.31 mol CO?

$$2.31 \text{ mol CO} \times \frac{2 \text{ mol NO}}{2 \text{ mol CO}} = \underline{2.31 \text{ mol NO}}$$

A mixture of hydrazine (N_2H_4) and hydrogen peroxide (H_2O_2) is used as a fuel for rocket engines. These substances react as follows:

$$N_2H_4(l) + 2H_2O_2(l) \rightarrow N_2(g) + 4H_2O(g)$$

How many mol of N_2H_4 will react to form 2.58 mol H_2O?

$$2.58 \text{ mol } H_2O \times \frac{1 \text{ mol } N_2H_4}{4 \text{ mol } H_2O} = \underline{0.645 \text{ mol } N_2H_4}$$

How many mol of H_2O_2 are needed to react with 1.25 mol N_2H_4?

$$1.25 \text{ mol } N_2H_4 \times \frac{2 \text{ mol } H_2O_2}{1 \text{ mol } N_2H_4} = \underline{2.50 \text{ mol } H_2O_2}$$

Chemical equations are also used to relate masses…

General steps:

1. write balanced chemical equation

2. convert mass to mol

3. obtain mol ratio

4. perform calculation

5. convert mol to mass

When baking soda ($NaHCO_3$) is heated, it decomposes, producing carbon dioxide. The carbon dioxide is responsible for the rising of the dough. How many grams of CO_2 are produced from 1.0 g of $NaHCO_3$?

$$2NaHCO_3(s) \rightarrow Na_2CO_3(s) + H_2O(g) + CO_2(g)$$

$$1.0\ \text{g NaHCO}_3 \times \frac{1\ \text{mol}}{84.01\ \text{g}} = 0.01\underline{1}9\ \text{mol NaHCO}_3$$

$$0.01\underline{1}9\ \text{mol NaHCO}_3 \times \frac{1\ \text{mol CO}_2}{2\ \text{mol NaHCO}_3} = 0.005\underline{9}5\ \text{mol CO}_2$$

$$0.005\underline{9}5\ \text{mol CO}_2 \times \frac{44.01\ \text{g}}{1\ \text{mol}} = \underline{0.26\ \text{g CO}_2}$$

Air bags inflate when sodium azide (NaN_3) rapidly decomposes into sodium metal and nitrogen gas. How many grams of nitrogen are produced when 130 g of NaN_3 decomposes?

$$2NaN_3(s) \rightarrow 2Na(s) + 3N_2(g)$$

$$130\ g\ NaN_3 \times \frac{1\ mol}{65.02\ g} = 1.\underline{9}9\ mol\ NaN_3$$

$$1.\underline{9}9\ mol\ NaN_3 \times \frac{3\ mol\ N_2}{2\ mol\ NaN_3} = 2.\underline{9}9\ mol\ N_2$$

$$2.\underline{9}9\ mol\ N_2 \times \frac{28.02\ g}{1\ mol} = \underline{84\ g\ N_2}$$

Limiting Reactant

When mixed in stoichiometric quantities, all reactants are used up in a chemical reaction

Ordinarily, reactants are not mixed in the exact ratio required

Reactants that are…

… not used up: excess reactants

… used up: limiting reactants

Limiting reactants limit the amount of product that can form

	$H_2(g)$	+	$Cl_2(g)$	$\rightarrow$	$2HCl(g)$
initial	1 mol		2 mol		0 mol
change	-1 mol		-1 mol		+2 mol
final	0 mol		1 mol		2 mol

H_2 is the limiting reactant… Cl_2 is the excess reactant

To determine which reactant is limiting...

1. Calculate amount of product formed by each reactant

2. Limiting reactant will produce smallest of calculated amounts

A 50.0 g sample of calcium carbonate reacts with 13.0 g of hydrochloric acid. How many grams of calcium chloride are produced?

$$CaCO_3(s) + 2HCl(aq) \rightarrow CaCl_2(aq) + CO_2(g) + H_2O(l)$$

$$50.0\ g\ CaCO_3 \times \frac{1\ mol}{100.09\ g} \times \frac{1\ mol\ CaCl_2}{1\ mol\ CaCO_3} = 0.500\ mol\ CaCl_2$$

$$13.0\ g\ HCl \times \frac{1\ mol}{36.46\ g} \times \frac{1\ mol\ CaCl_2}{2\ mol\ HCl} = 0.178\ mol\ CaCl_2 \quad (LR)$$

$$0.178\ mol\ CaCl_2 \times \frac{110.98\ g}{1\ mol} = \underline{19.8\ g\ CaCl_2} \quad (TY)$$

Theoretical yield is amount of product formed when limiting reactant is completely consumed

How many grams of calcium carbonate are in excess?

$$13.0\ g\ HCl \times \frac{1\ mol}{36.46\ g} = 0.35\underline{6}5\ mol\ HCl \quad \text{(used)}$$

$$0.35\underline{6}5\ mol\ HCl \times \frac{1\ mol\ CaCO_3}{2\ mol\ HCl} \times \frac{100.09\ g}{1\ mol} = 17.8\ g\ CaCO_3 \quad \text{(used)}$$

$$50.0\ g\ CaCO_3 - 17.8\ g\ CaCO_3 = \underline{32.2\ g\ CaCO_3} \quad \text{(excess)}$$

How many grams of silver phosphate can be formed from mixing 1.2 g of silver nitrate and 4.8 g of sodium phosphate?

$$3AgNO_3(aq) + Na_3PO_4(aq) \rightarrow Ag_3PO_4(s) + 3NaNO_3(aq)$$

$$1.2 \text{ g } AgNO_3 \text{ x } \frac{1 \text{ mol}}{169.88 \text{ g}} \text{ x } \frac{1 \text{ mol } Ag_3PO_4}{3 \text{ mol } AgNO_3} = 0.002\underline{3}5 \text{ mol } Ag_3PO_4 \quad \text{(LR)}$$

$$4.8 \text{ g } Na_3PO_4 \text{ x } \frac{1 \text{ mol}}{163.94 \text{ g}} \text{ x } \frac{1 \text{ mol } Ag_3PO_4}{1 \text{ mol } Na_3PO_4} = 0.02\underline{9}2 \text{ mol } Ag_3PO_4$$

$$0.002\underline{3}5 \text{ mol } Ag_3PO_4 \text{ x } \frac{418.58 \text{ g}}{1 \text{ mol}} = 0.98 \text{ g } Ag_3PO_4 \quad \text{(TY)}$$

Actual yield is the amount of product that is actually obtained

Percent yield is the percent of theoretical yield that is actually obtained

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

What is the percent yield if only 0.82 g Ag_3PO_4 are obtained?

$$\% \text{ Yield} = \frac{0.82 \text{ g}}{0.98 \text{ g}} \times 100$$

$$= \underline{84\% \text{ Yield}}$$

Aluminum and oxygen react to form aluminum oxide. In an experiment 75.0 g of Al and 200.0 g of O_2 produce 125 g of Al_2O_3.

$$4Al(s) + 3O_2(g) \rightarrow 2Al_2O_3(s)$$

What is the theoretical yield (in g) of Al_2O_3?

$$75.0\ g\ Al \times \frac{1\ mol}{26.98\ g} \times \frac{2\ mol\ Al_2O_3}{4\ mol\ Al} = 1.3\underline{8}9\ mol\ Al_2O_3 \quad (LR)$$

$$200.0\ g\ O_2 \times \frac{1\ mol}{32.00\ g} \times \frac{2\ mol\ Al_2O_3}{3\ mol\ O_2} = 4.16\underline{6}6\ mol\ Al_2O_3$$

$$1.3\underline{8}9\ mol\ Al_2O_3 \times \frac{101.96\ g}{1\ mol} = \underline{142\ g\ Al_2O_3} \quad (TY)$$

What is the percent yield of Al_2O_3?

$$\% \text{ Yield} = \frac{125 \text{ g}}{142 \text{ g}} \text{ x } 100 = \underline{88.0 \% \text{ Yield}}$$

How many grams of O_2 are in excess?

$$75.0 \text{ g Al x } \frac{1 \text{ mol}}{26.98 \text{ g}} = 2.7\underline{7}9 \text{ mol Al} \quad \text{(used)}$$

$$2.7\underline{7}9 \text{ mol Al x } \frac{3 \text{ mol } O_2}{4 \text{ mol Al}} \text{ x } \frac{32.00 \text{ g}}{1 \text{ mol}} = 66.\underline{7}1 \text{ g } O_2 \quad \text{(used)}$$

$$200.0 \text{ g } O_2 - 66.\underline{7}1 \text{ g } O_2 = \underline{133.3 \text{ g } O_2} \quad \text{(excess)}$$

Heat of Reaction

Bonds are broken and formed in chemical reactions…

- Energy absorbed in breaking bonds, and released in forming bonds
- Energy balance determines net loss or net gain of energy

The energy change in a reaction is the <u>heat of reaction</u>

- Heat of reaction is also known as enthalpy change (ΔH)
  - ΔH is +: endothermic
  - ΔH is -: exothermic

Endothermic reactions proceed with net gain of energy

energy is “reactant”… requires continuous input of energy

$$N_2(g) + O_2(g) + 181\ kJ \rightarrow 2NO(g)\ (+181\ kJ)$$

the surroundings cool down

Exothermic reactions proceed with net loss of energy

energy is “product”… energy continuously released

$$C(s) + O_2(g) \rightarrow CO_2(g) + 393\ kJ\quad (-393\ kJ)$$

the surroundings warm up

How many kilojoules of energy are released when 10.0 g of hydrogen react with an excess of oxygen?

$$2H_2(g) + O_2(g) \rightarrow 2H_2O(g) \qquad \Delta H = -484\ kJ$$

$$10.0\ g\ H_2 \times \frac{1\ mol\ H_2}{2.016\ g\ H_2} \times \frac{-484\ kJ}{2\ mol\ H_2} = \underline{-12\bar{0}0\ kJ}$$

How many grams of water are produced in a reaction that releases 36.3 kJ of energy?

$$-36.3\ kJ \times \frac{2\ mol\ H_2O}{-484\ kJ} \times \frac{18.02\ g\ H_2O}{1\ mol\ H_2O} = \underline{2.70\ g\ H_2O}$$