Chemical Equations and Stoichiometry

Topics:

- Equation Writing and Balancing
  - Stoichiometry
  - Coefficients
  - Mass-Mole Relationships
- Limiting Reagents
- Percent Yield
- Quantitative Analysis
  - Combustion (Revisited)
  - Titration / Mineral Analysis

Writing and Balancing Chemical Equations

Reactants → Products

(e.g. A + B → C + D)

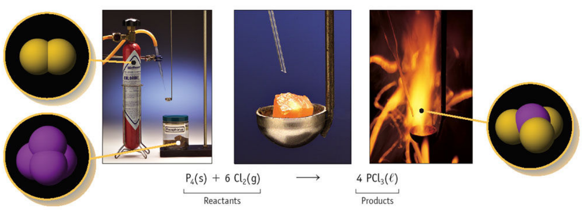
Mass must be conserved in the chemical reaction (Conservation of Mass – Antoine Lavoisier)

The number and type of atoms on each side of the reaction equation must be balanced.

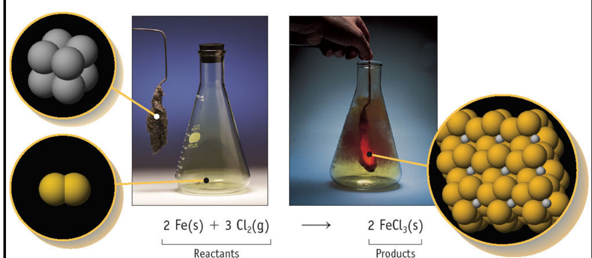
Chemical equations MUST be balanced by coefficients.

Once the chemical formulas for the reactants and products are determined you MUST NOT change any subscripts, nor can you balance the equation by putting coefficients in the MIDDLE of a compound.

Formation of a Molecular Compound



Formation of an Ionic Compound



Coefficients multiply through to every element in the compounds.

Ex. $CaO_{(s)} + 2NH_4Cl_{(s)} \rightarrow 2NH_{3(g)} + H_2O_{(g)} + CaCl_{2(s)}$

In the product, the 2 in front of NH_3 affects both the N and the H; i.e. 2 N and 6 H

Coefficients tell you the mole ratio NOT mass ratio of the reaction components.

Ex. In the equation above; 1 mole of CaO reacts with 2 moles of NH_4Cl to produce 2 moles of NH_3, and 1 mole each of H_2O and $CaCl_2$

All masses must be converted to moles before setting up mole ratios

It is a good idea to take inventory on the elements in the reaction.

The symbols (aq), (l), (g), (s) are used to designate aqueous, liquid, gas and solid, respectively.

Practice Problems: Balance the Following Reactions

____$BaCl_{2(aq)}$ + _2_$AgNO_{3(aq)}$ → _2_$AgCl_{(s)}$ + ____$Ba(NO_3)_{2(aq)}$

_2_$SO_{2(g)}$ + _2_$CaCO_{3(s)}$ + ____$O_{2(g)}$ → _2_$CaSO_{4(s)}$ + _2_$CO_{2(g)}$

___$NiCO_{3(s)}$ + _2_$HNO_{3(aq)}$ → ___$Ni(NO_3)_{2(aq)}$ + ___ $CO_{2(g)}$ + ___$H_2O_{(l)}$

Often you may have to translate a description of the reaction into a chemical reaction equation before balancing.

Sample Problems: Write and balance the following reactions

1. **Sodium phosphate reacts with calcium chloride to yield calcium phosphate and sodium chloride.**

$$2Na_3PO_4 + 3CaCl_2 \rightarrow Ca_3(PO_4)_2 + 6NaCl$$

2. **Copper and sulfuric acid react to yield cupric sulfate, water and sulfur dioxide.**

$$Cu + 2H_2SO_4 \rightarrow CuSO_4 + 2H_2O + SO_2$$

Stoichiometry: Mole-Mass Relationships

Chemical reaction equations are written in terms of mole ratios.

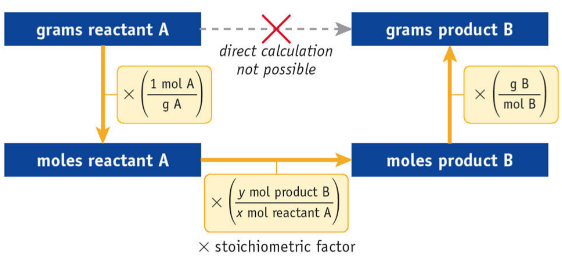
In order to solve quantitative problems using these equations, all values representing amounts of substances must be converted to moles via the substance's molar mass (or molarity or standard molar volume)

Moles of substance = grams / molar mass (g/mol)

Grams of substance = moles * molar mass (g/mol)

3 Step Process:

1. Convert grams to moles
2. Compare mole ratios
3. Convert moles to grams



What is stoichiometry used for?

1. Calculating amounts of reactants required for a reaction.
2. Calculating amounts of product(s) produced.
3. Determining if you have enough of one reactant relative to another (limiting reagent)
4. Comparing the amount of product actually produced (actual yield) with the amount based on the stoichiometry of the reaction (theoretical yield). From this the percent yield can be determined.

Percent Yield = (Actual Yield / Theoretical Yield) x 100%

Sample Problems: Solve the following questions

1. **Calculate the mass of hydrogen required to react with 15.40g of oxygen to produce water vapor.**

$2H_2 + O_2 \rightarrow 2H_2O$
15.40g O_2 / 32.00g/mol = .41825mol O_2
.41825mol O_2 (2mol H_2 / 1mol O_2) = .9625mol H_2
.9625mol H_2 (2.016g/mol) = **1.940g H_2**

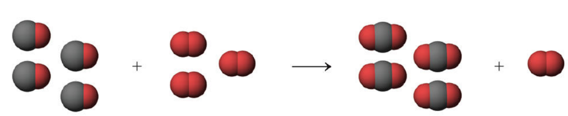
2. **Determine how much ferric chloride can be produced from 22.35g of chlorine gas and excess iron.**

$2Fe + 3Cl_2 \rightarrow 2FeCl_3$
22.35g Cl_2 / 70.90g/mol = .3152mol Cl_2
.3152mol Cl_2 (2mol $FeCl_3$ / 3mol Cl_2) = .2102mol $FeCl_3$
.2102mol $FeCl_3$ (162.2g/mol) = **34.09g $FeCl_3$**

Limiting Reagents: The reactant that you run out of first. Limits the amount of product that can be formed.

Not always the lesser mass of reactant nor the lesser number of moles!

Limiting reagents must be determined stoichiometrically.



$$2CO + O_2 \rightarrow 2CO_2$$

A clue that a question is a limiting reagent problem is that specific masses of all reactants are given in the problem.

Sample Problems: Solve the following questions

1. **Urea [$(NH_2)_2CO$] (60.06g/mol) is prepared by reacting ammonia with carbon dioxide. The other product is water. In one process, 637.2g of ammonia (17.03g/mol) are allowed to react with 1142g of carbon dioxide (44.01g/mol).**

   a) Which of the two reactants is the limiting reagent?

   b) Calculate the mass of $(NH_2)_2CO$ formed.

   c) How much of the excess reagent (in grams) is left at the end of the reaction.

$2NH_3 + CO_2 \rightarrow (NH_2)_2CO + H_2O$
637.2gNH_3 1142gCO_2
Mol NH_3 = 637.2g / 17.03g/mol = 37.41632 = 37.42mol NH_3
Mol CO_2 = 1142g / 44.01g/mol = 25.94865 = 25.95mol CO_2

a) Mole ratio of NH_3 to CO_2 is 2:1 so by the moles above NH_3 limits

b) Use limiting reagent to calculate products
37.42mol NH_3 (1mol $(NH_2)_2CO$ / 2mol NH_3) = 18.7082mol $(NH_2)_2CO$
18.7082mol $(NH_2)_2CO$ (60.06g/mol) = 1123.6g = 1124g $(NH_2)_2CO$

c) Moles CO_2 left = 25.994865mol – (37.41632mol / 2) = 7.24049mol CO_2
7.24049mol CO_2 (44.01g/mol) = 318.654g = 318.7g CO_2 remains

Sample Problem:

The reaction between aluminum and iron(II)oxide can generate temperatures approaching 3,000°C and is used in welding metals.

$2Al + Fe_2O_3 \rightarrow Al_2O_3 + 2Fe$

In one process, 124g of Al (26.98g/mol) are reacted with 601g of Fe_2O_3 (159.69g/mol).

a) Calculate the mass (in grams) of Al_2O_3 (101.96g/mol) formed.

b) How much of the excess reagent is left at the end of the reaction?

124g Al 601gFe_2O_3

Mol Al = 124g / 26.98g/mol = 4.5959 = 4.60mol Al
mol Fe_2O_3 601g / 159.69g/mol = 3.7635 = 3.76mol Fe_2O_3

Since Al combines with Fe_2O_3 in a 2:1 ratio
The results above show Al limits

4.60mol Al (1mol Al_2O_3 / 2mol Al) = 2.297998 = 2.30mol Al_2O_3
2.30mol Al_2O_3 (101.96g/mol) = 234.3039 = 234g Al_2O_3

b) Excess Fe_2O_3
3.76mol Fe_2O_3 – (4.60mol Al / 2) = 1.46559mol Fe_2O_3
1.46559mol Fe_2O_3 (159.69g/mol) = 234.04 = 234g Fe_2O_3

Percent Yield Sample Problem:

Industrially, vanadium metal (50.94g/mol), which is used in steel alloys, can be obtained by reacting vanadium(V)oxide (181.88g/mol) with calcium (40.08g/mol) at high temperatures. The other product is calcium oxide (56.08g/mol).

If 1.54x10^{3}g of vanadium(V)oxide is reacted with 1.96x10^{3}g of Ca

a) Calculate the theoretical yield of V.

b) Calculate the percent yield if 803g of V are obtained.

Answer:

$V_2O_5 + 5Ca \rightarrow 5CaO + 2V$

Mol V_2O_5 = 1.54x10^{3}g / 181.88g/mol = 8.467mol (8.47)
Mol Ca = 1.96x10^{3}g / 40.08g/mol = 48.902mol (48.9)

V_2O_5 limits b/c 8.467 (5mol Ca / 1mol V_2O_5) = 42.34mol
8.467mol (2mol V / 1mol V_2O_5) = 16.9342mol V
16.9342mol V (50.94g/mol) = 862.63 = 863g V

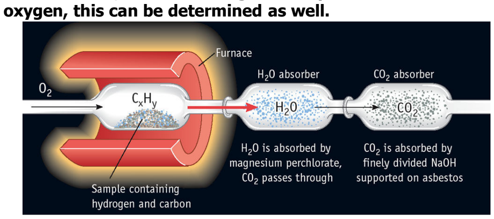
b) 803/863 = .93087 = 93.1%

Percent Yield Sample Problem:

Titanium (47.88g/mol) can be recovered from titanium(IV)chloride (189.68g/mol) by reacting it with magnesium in a single replacement reaction that takes place at between 950-1150°C. If the reaction is known to have an 87.5% yield, how much titanium(IV)chloride (in kg) should be reacted with excess magnesium in order to produce 185.6kg of titanium?

Answer:
$2Mg + TiCl_4 \rightarrow 2MgCl_2 + Ti$
185.6kg must represent the 87.5% yield (actual)
Theoretical = 185.6 / .875 = 212kg Ti (212.114…)
2.12×10^5g / 47.88g/mol = 4.43×10^3mol Ti
4.43×10^3mol Ti (1mol $TiCl_4$ / 1mol Ti) = 4.43×10^3mol $TiCl_4$
4.43×10^3mol $TiCl_4$ (189.68g $TiCl_4$ / 1mol) = 840305.7g = 8.40×10^2kg $TiCl_4$

<u>Combustion Analysis (Revisited)</u>: By analyzing the hydrogen content in the H_2O absorber and the carbon content in the CO_2 absorber, the empirical formula of a hydrocarbon can be deduced. If the initial sample mass is also known, then if the original compound contained oxygen, this can be determined as well.



In the last chapter, we determined this through mass percent composition. This chapter shows that it can also be done using mole ratios between reactants and products. The general formula is still $C_xH_y + O_2 \rightarrow CO_2 + H_2O$ (unbalanced)

Example Problem: A 50.00g sample of a hydrocarbon containing C, H and O is combusted to produce 68.68g of CO_2 and 56.23g H_2O. What is the empirical formula for the compound. Try to use stoichiometry for practice.

Answer:
Moles of CO_2 = 68.68g (1mol CO_2 / 44.01g) = 1.561mol CO_2
1.561mol CO_2 (1mol C / 1mol CO_2) = <u>1.561mol C</u>
1.561mol C (12.01g/mol) = 18.75g C

Moles of H_2O = 56.23g (1mol H_2O / 18.016g) = 3.121mol H_2O
3.121mol H_2O (2mol H / 1mol H_2O) = <u>6.242mol H</u>
6.242mol H (1.008g/mol) = 6.292g H

Grams of O = 50.00g – 18.75g – 6.292g = 24.958gO = 24.96gO
24.96gO (1mol O / 16.00g) = <u>1.560mol O</u>

$C_{1.561}H_{6.242}O_{1.560}$
$C_{1.561/1.560}H_{6.242/1.560}O_{1.560/1.560}$
CH_4O

<u>Titration:</u> Using a substance of known concentration to analyze a substance of unknown quantity or mass if the chemical equation is known.

<u>Mineral Analysis:</u> Determining the amount of a particular substance in a mineral by reacting it with one or more other substances in a methodical process from which the unknown quantity can be determined.

<u>Sample Problem</u>:

<u>Mineral Analysis</u>:
Limestone is a sedimentary rock composed largely of the mineral calcite (calcium carbonate: $CaCO_3$ (100.09g/mol)). To test the purity of the calcium carbonate, a sample of the mineral is reacted with hydrochloric acid to produce calcium chloride, carbon dioxide and water. If a 15.70g sample of calcite is reacted with excess hydrochloric acid and 16.89g of calcium chloride (110.98g/mol) are produced, what is the percent purity of the calcium carbonate in the limestone?

Answer:

15.70g sample of calcite

$CaCO_3 + 2HCl \rightarrow CaCl_2 + CO_2 + H_2O$

16.89g$CaCl_2$ / 110.98g/mol = .15219mol $CaCl_2$

.15219mol $CaCl_2$ (1mol $CaCO_3$ / 1mol $CaCl_2$) = .15219mol $CaCO_3$

.15219mol $CaCO_3$ (100.09g/mol) = 15.2327g

15.23 / 15.70 = .9701 = 97.01% pure