1. STOICHIOMETRY INVOLVING ONLY PURE SUBSTANCES

For all chemical reactions, the balanced chemical equation gives the mole ratios of reactants and products. If we are dealing with pure chemicals, the molar mass allows us to convert the mass of a reactant or product into moles. Consider the reaction shown below.

\[
\text{Ca}_3\text{N}_2(s) + 6\text{H}_2\text{O}(l) \rightarrow 2\text{NH}_3(g) + 3\text{Ca(OH)}_2(s)
\]

<table>
<thead>
<tr>
<th>mole ratio</th>
<th>1 : 6 : 2 : 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>molar mass (g/mole)</td>
<td>148.3 : 18.0 : 17.0 : 74.1</td>
</tr>
</tbody>
</table>

For this reaction, 1 mole of \(\text{Ca}_3\text{N}_2\) will react with 6 moles of \(\text{H}_2\text{O}\) to produce 2 moles of \(\text{NH}_3\) and 3 moles of \(\text{Ca(OH)}_2\). Therefore, for this reaction 1 mole \(\text{Ca}_3\text{N}_2\) \(\equiv\) 6 moles \(\text{H}_2\text{O}\). Similar equivalences will apply to other pairs of reactants and/or products. For example, 6 moles \(\text{H}_2\text{O}\) \(\equiv\) 2 moles \(\text{NH}_3\). As discussed before, each equivalence will give two conversion factors.

(a) Calculate the number of moles of \(\text{H}_2\text{O}\) that will react with 2.5 moles of \(\text{Ca}_3\text{N}_2\).

\[
\text{moles H}_2\text{O} = 2.5 \text{ moles Ca}_3\text{N}_2 \times \frac{6 \text{ moles H}_2\text{O}}{1 \text{ mole Ca}_3\text{N}_2} = 15 \text{ moles H}_2\text{O}
\]

(b) How many moles of \(\text{NH}_3\) can be made by the reaction of 0.75 mole of \(\text{Ca}_3\text{N}_2\) with an excess of \(\text{H}_2\text{O}\)? (Ans. 1.5 mole)

(c) How many moles of \(\text{H}_2\text{O}\) are needed to make 12 moles of \(\text{NH}_3\)? (Ans. 36 moles)

(d) Calculate the mass of \(\text{Ca(OH)}_2\) that can be formed from the reaction of 10.0 g of \(\text{Ca}_3\text{N}_2\) with an excess of \(\text{H}_2\text{O}\).

\[
\text{moles Ca}_3\text{N}_2 = 10.0 \text{ g Ca}_3\text{N}_2 \times \frac{1 \text{ mole Ca}_3\text{N}_2}{148.3 \text{ g Ca}_3\text{N}_2} = 0.06743 \text{ mole}
\]

\[
\text{moles Ca(OH)}_2 = 0.06743 \text{ mole Ca}_3\text{N}_2 \times \frac{3 \text{ moles Ca(OH)}_2}{1 \text{ mole Ca}_3\text{N}_2} = 0.2023 \text{ mole}
\]

\[
\text{mass Ca(OH)}_2 = 0.2023 \text{ mole} \times \frac{74.1 \text{ g Ca(OH)}_2}{1 \text{ mole Ca(OH)}_2} = 15.0 \text{ g}
\]

(e) What mass of \(\text{NH}_3\) can be formed from the reaction of 23.5 g of \(\text{H}_2\text{O}\) with an excess of \(\text{Ca}_3\text{N}_2\)? (Ans. 7.40 g)

(f) What mass of \(\text{H}_2\text{O}\) is needed to make 454 g of \(\text{Ca(OH)}_2\)? (Ans. 221 g)

(g) What volume of \(\text{H}_2\text{O}\) is needed to react completely with 45.0 g of \(\text{Ca}_3\text{N}_2\)? (Ans. 32.8 mL)
2. **THEORETICAL, ACTUAL AND PERCENT YIELD**

The amount of a product calculated for a reaction is only a theoretical amount and is therefore called the theoretical yield. When a reaction is actually performed, the amount of product obtained (or isolated) (the actual yield) is usually less than the theoretical yield. The percent yield gives the actual yield as a percentage of the theoretical yield.

\[
\text{percent yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100
\]

(h) If only 6.85 g of NH\textsubscript{3} was obtained from the reaction in (e), what is the percent yield of the reaction? (Ans. 92.6%)

(i) If the percent yield of Ca(OH)\textsubscript{2} from Ca\textsubscript{3}N\textsubscript{2} is 93.0%, what mass of Ca\textsubscript{3}N\textsubscript{2} must be used to obtain 66.0 g of Ca(OH)\textsubscript{2}? (HINT: Use the percent yield to calculate the theoretical yield and then use the theoretical to calculate the amount of reactant needed). (Ans. 47.3 g)

3. **STOICHIOMETRY AND PERCENT PURITY**

Many samples of chemicals are not pure. We can define percent purity as

\[
\frac{\text{mass of pure compound in the impure sample}}{\text{total mass of impure sample}} \times 100
\]

If an impure sample of a chemical of known percent purity is used in a chemical reaction, the percent purity has to be used in stoichiometric calculations. Conversely, the percent purity of an impure sample of a chemical of unknown percent purity can be determined by reaction with a pure compound as in an acid-base titration. Percent purity can also be determined, in theory, by measuring the amount of product obtained from a reaction. This latter approach, however, assumes a 100% yield of the product.

Consider the reaction of magnesium hydroxide with phosphoric acid.

\[
3\text{Mg(OH)}_2 + 2\text{H}_3\text{PO}_4 \rightarrow \text{Mg}_3(\text{PO}_4)_2 + 6\text{H}_2\text{O}
\]

(a) Calculate the mass of Mg\textsubscript{3}(PO\textsubscript{4})\textsubscript{2} that will be formed (assuming a 100% yield) from the reaction of 15.0 g of 92.5% Mg(OH)\textsubscript{2} with an excess of H\textsubscript{3}PO\textsubscript{4}.

\[
\text{mass Mg(OH)}_2 = 15.0 \times 0.925 = 13.875 \text{ g}
\]

\[
\text{mass Mg}_3(\text{PO}_4)_2 = 13.875 \text{ g Mg(OH)}_2 \times \frac{1 \text{ mole Mg(OH)}_2}{58.3 \text{ g Mg(OH)}_2} \times \frac{1 \text{ mole Mg}_3(\text{PO}_4)_2}{3 \text{ moles Mg(OH)}_2} \times \frac{262.9 \text{ g Mg}_3(\text{PO}_4)_2}{1 \text{ mole Mg}_3(\text{PO}_4)_2} = 20.9 \text{ g Mg}_3(\text{PO}_4)_2
\]
(b) Calculate the mass of 88.5% Mg(OH)_2 needed to make 127 g of Mg_3(PO_4)_2, assuming a 100% yield.

\[
\text{mass Mg(OH)}_2 = 127 \text{ g Mg}_3(\text{PO}_4)_2 \times \frac{1 \text{ mole Mg}_3(\text{PO}_4)_2}{262.9 \text{ g Mg}_3(\text{PO}_4)_2} \times \frac{3 \text{ moles Mg(OH)}_2}{1 \text{ mole Mg}_3(\text{PO}_4)_2} \times \frac{58.3 \text{ g Mg(OH)}_2}{1 \text{ mole Mg(OH)}_2} \\
= 84.49 \text{ g Mg(OH)}_2.
\]

\[
\text{mass 88.5% Mg(OH)}_2 = 84.49 \text{ g Mg(OH)}_2 \times \frac{100 \text{ g } 88.5\% \text{ Mg(OH)}_2}{88.5 \text{ g Mg(OH)}_2} = 95.5 \text{ g}
\]

(c) Calculate the percent purity of a sample of Mg(OH)_2 if titration of 2.568 g of the sample required 38.45 mL of 0.6695 M H_3PO_4.

\[
\text{mass Mg(OH)}_2 = 38.45 \text{ mL H}_3\text{PO}_4 \times \frac{0.6695 \text{ mole H}_3\text{PO}_4}{1000 \text{ mL H}_3\text{PO}_4} \times \frac{3 \text{ moles Mg(OH)}_2}{2 \text{ moles H}_3\text{PO}_4} \times \frac{58.3 \text{ g Mg(OH)}_2}{1 \text{ mole Mg(OH)}_2} \\
= 2.251 \text{ g Mg(OH)}_2. \text{ Percent purity} = \frac{2.251}{2.568} \times 100 = 87.7\%
\]

Consider the reaction \(4\text{PH}_3 + 8\text{O}_2 \rightarrow \text{P}_4\text{O}_{10} + 6\text{H}_2\text{O}\)

(a) Calculate the theoretical yield of \(\text{P}_4\text{O}_{10}\) from the reaction of 15.0 g of 88.0% PH_3 with excess \text{O}_2. (Ans. 27.6 g)

(b) What mass of 94.0% PH_3 is needed to make 500.0 g of \(\text{P}_4\text{O}_{10}\), assuming a 100% yield? (Ans. 255 g)

(c) Calculate the percent purity of a sample of PH_3 if 55.0 g of the impure sample reacted with excess \text{O}_2 to produce 39.3 g of \text{H}_2\text{O}. (Ans. 90.0%)

(d) Calculate the percent purity of a sample of Al_2O_3 if 0.1104 g of the impure sample required 27.28 mL of 0.1046 M H_2SO_4 for complete titration. The reaction is given below. (Ans. 87.88%)

\[
\text{Al}_2\text{O}_3(s) + 3\text{H}_2\text{SO}_4(aq) \rightarrow \text{Al}_2(\text{SO}_4)_3(aq) + 3\text{H}_2\text{O}(l)
\]
4. LIMITING REACTANTS

(a) Consider the reaction \( \text{Ca}_3\text{N}_2 + 6\text{H}_2\text{O} \rightarrow 2\text{NH}_3 + 3\text{Ca(OH)}_2 \)

For the reaction of 20.0 g of \( \text{Ca}_3\text{N}_2 \) with 16.0 g of \( \text{H}_2\text{O} \),
(1) calculate the theoretical yield of \( \text{Ca(OH)}_2 \),
(2) determine the limiting reactant, and
(3) calculate the mass of the excess reactant left over.

**Solution:**

From \( \text{Ca}_3\text{N}_2 \): mass of \( \text{Ca(OH)}_2 \) = \( 20.0 \text{ g } \text{Ca}_3\text{N}_2 \times \frac{3 \times 74.1 \text{ g } \text{Ca(OH)}_2}{148.3 \text{ g } \text{Ca}_3\text{N}_2} = 30.0 \text{ g} \)

From \( \text{H}_2\text{O} \): mass of \( \text{Ca(OH)}_2 \) = \( 16.0 \text{ g } \text{H}_2\text{O} \times \frac{3 \times 74.1 \text{ g } \text{Ca(OH)}_2}{6 \times 18.0 \text{ g } \text{H}_2\text{O}} = 32.9 \text{ g} \)

(1) the theoretical yield of \( \text{Ca(OH)}_2 \) is 30.0 g.
(2) the limiting reactant is \( \text{Ca}_3\text{N}_2 \).

(3) the mass of \( \text{H}_2\text{O} \) reacted = \( 20.0 \text{ g } \text{Ca}_3\text{N}_2 \times \frac{6 \times 18.0 \text{ g } \text{H}_2\text{O}}{148.3 \text{ g } \text{Ca}_3\text{N}_2} = 14.6 \text{ g} \)

mass of \( \text{H}_2\text{O} \) left over = (16.0 - 14.6) g = 1.4 g

(b) For the reaction \( 4\text{PH}_3 + 8\text{O}_2 \rightarrow \text{P}_4\text{O}_{10} + 6\text{H}_2\text{O} \) calculate (1) the theoretical yield of \( \text{P}_4\text{O}_{10} \), and (2) the mass of the excess reactant left over when 35.0 g of \( \text{PH}_3 \) were reacted with 60.0 g of \( \text{O}_2 \). [Ans. (1) 66.6 g \( \text{P}_4\text{O}_{10} \), (2) 3.1 g \( \text{PH}_3 \)]

(c) Consider the reaction \( 3\text{NaBH}_4 + 4\text{BF}_3 \rightarrow 3\text{NaBF}_4 + 2\text{B}_2\text{H}_6 \)

The reaction was carried out using 78.0 g of \( \text{NaBH}_4 \) and 172.0 g of \( \text{BF}_3 \). Calculate
(1) the theoretical yield of \( \text{B}_2\text{H}_6 \), and
(2) the mass of the excess reactant left over.
[Ans. (1) 35.0 g \( \text{B}_2\text{H}_6 \), (2) 6.1 g \( \text{NaBH}_4 \)]
5. STOICHIOMETRY AND THERMOCHEMICAL EQUATIONS

In all chemical reactions, heat is either released (or evolved, or liberated) (exothermic reactions) or absorbed (or used) (endothermic reactions). When heat is released, heat can be treated (at the CHEM 094 level; a more rigorous treatment is used at the CHEM 105 and higher levels) as a product of the reaction. When heat is absorbed, it must be supplied and can be treated as a reactant in the reaction.

An example of an exothermic reaction is the combustion of methane (\( \text{CH}_4 \); the main constituent of natural gas). The equation for the reaction is given below.

\[
\text{CH}_4(g) + 2\text{O}_2(g) \rightarrow \text{CO}_2(g) + 2\text{H}_2\text{O}(l) + 890 \text{ kJ}
\]

An example of an endothermic reaction is the reaction of nitrogen with oxygen to produce \( \text{N}_2\text{O} \). This reaction can be written

\[
2\text{N}_2(g) + \text{O}_2(g) + 163 \text{ kJ} \rightarrow 2\text{N}_2\text{O}(g)
\]

Chemical equations which include the amount of heat released or absorbed are called thermochemical equations and must have the physical states of all reactants and products specified. In these equations, the amount of heat released or absorbed are for the number of moles of reactants and products given in the equation. For example, when 1 mole of \( \text{CH}_4(g) \) reacts with \( \text{O}_2(g) \) to produce 1 mole of \( \text{CO}_2(g) \) and 2 moles of \( \text{H}_2\text{O}(l) \), 890 kJ of heat are released. [Note that the reaction of 1 mole of \( \text{CH}_4(g) \) with \( \text{O}_2(g) \) to produce 1 mole of \( \text{CO}_2(g) \) and 2 moles of \( \text{H}_2\text{O}(g) \) would produce less heat because heat is needed to convert \( \text{H}_2\text{O}(l) \) (liquid water) to \( \text{H}_2\text{O}(g) \) (water vapour)]. Hence, thermochemical equations can be treated as other equations for stoichiometric calculations.

**Example**

The reaction for the combustion of ethane gas (\( \text{C}_2\text{H}_6 \)) is given below.

\[
2\text{C}_2\text{H}_6(g) + 7\text{O}_2(g) \rightarrow 4\text{CO}_2(g) + 6\text{H}_2\text{O}(l) + 3119 \text{ kJ}
\]

(a) Calculate how much heat is released (given off) when 555 g of ethane are reacted.

\[
555 \text{ g } \text{C}_2\text{H}_6 \times \frac{1 \text{ mole } \text{C}_2\text{H}_6}{30.0 \text{ g } \text{C}_2\text{H}_6} \times \frac{3119 \text{ kJ}}{2 \text{ moles } \text{C}_2\text{H}_6} = 2.89 \times 10^4 \text{ kJ}
\]

(b) Calculate how much water is produced when 955 kJ are released.

\[
955 \text{ kJ} \times \frac{6 \text{ moles } \text{H}_2\text{O}}{3119 \text{ kJ}} \times \frac{18.0 \text{ g } \text{H}_2\text{O}}{1 \text{ mole } \text{H}_2\text{O}} = 33.1 \text{ g H}_2
\]