**CHEQ 1094 STOICHIOMETRY**

## 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.

| | $Ca_3N_2(s)$ | + | $6H_2O(l)$ | $\rightarrow$ | $2NH_3(g)$ | + | $3Ca(OH)_2(s)$ |
|---|---|---|---|---|---|---|---|
| mole ratio | 1 | : | 6 | : | 2 | : | 3 |
| molar mass (g/mole) | 148.3 | | 18.0 | | 17.0 | | 74.1 |

For this reaction, 1 mole of $Ca_3N_2$ will react with 6 moles of $H_2O$ to produce 2 moles of $NH_3$ and 3 moles of $Ca(OH)_2$. Therefore, for this reaction 1 mole $Ca_3N_2 \equiv 6$ moles $H_2O$. Similar equivalences will apply to other pairs of reactants and/or products. For example, 6 moles $H_2O \equiv 2$ moles $NH_3$. As discussed before, each equivalence will give two conversion factors.

(a) Calculate the number of moles of $H_2O$ that will react with 2.5 moles of $Ca_3N_2$.

*Solution*:

$$\text{moles } H_2O = \underbrace{2.5 \text{ moles } Ca_3N_2}_{\textbf{given}} \times \underbrace{\frac{6 \text{ moles } H_2O}{1 \text{ mole } Ca_3N_2}}_{\textbf{mole ratio}} = 15 \text{ moles } H_2O$$

(b) How many moles of $NH_3$ can be made by the reaction of 0.75 mole of $Ca_3N_2$ with an excess of $H_2O$? (*Ans*. 1.5 mole)

(c) How many moles of $H_2O$ are needed to make 12 moles of $NH_3$? (*Ans*. 36 moles)

(d) Calculate the mass of $Ca(OH)_2$ that can be formed from the reaction of 10.0 g of $Ca_3N_2$ with an excess of $H_2O$.

*Solution:* $\text{moles } Ca_3N_2 = 10.0 \text{ g } Ca_3N_2 \times \dfrac{1 \text{ mole } Ca_3N_2}{148.3 \text{ g } Ca_3N_2} = 0.06743 \text{ mole}$

$$\text{moles } Ca(OH)_2 = 0.06743 \text{ mole } Ca_3N_2 \times \frac{3 \text{ moles } Ca(OH)_2}{1 \text{ mole } Ca_3N_2} = 0.2023 \text{ mole}$$

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

(e) What mass of $NH_3$ can be formed from the reaction of 23.5 g of $H_2O$ with an excess of $Ca_3N_2$? (*Ans*. 7.40 g)

(f) What mass of $H_2O$ is needed to make 454 g of $Ca(OH)_2$? (*Ans*. 221 g)

(g) What volume of $H_2O$ is needed to react completely with 45.0 g of $Ca_3N_2$? (*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.

$$\textbf{percent yield} = \frac{\textbf{actual yield}}{\textbf{theoretical yield}}\ \textbf{x 100}$$

(h) If only 6.85 g of $NH_3$ was obtained from the reaction in (e), what is the percent yield of the reaction? (*Ans*. 92.6%)

(i) If the percent yield of $Ca(OH)_2$ from $Ca_3N_2$ is 93.0%, what mass of $Ca_3N_2$ must be used to obtain 66.0 g of $Ca(OH)_2$? (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

$$\frac{\text{mass of pure compound in the impure sample}}{\text{total mass of impure sample}}\ \text{x}\ 100$$

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.

$$3Mg(OH)_2 \quad + \quad 2H_3PO_4 \quad \rightarrow \quad Mg_3(PO_4)_2 \quad + \quad 6H_2O$$

(a) Calculate the mass of $Mg_3(PO_4)_2$ that will be formed (assuming a 100% yield) from the reaction of 15.0 g of 92.5% $Mg(OH)_2$ with an excess of $H_3PO_4$.

mass $Mg(OH)_2$ = 15.0 x 0.925 = 13.875 g
mass $Mg_3(PO_4)_2$ =

$$13.875\text{ g } Mg(OH)_2 \text{ x } \frac{1\text{ mole } Mg(OH)_2}{58.3\text{ g } Mg(OH)_2} \text{ x } \frac{1\text{ mole } Mg_3(PO_4)_2}{3\text{ moles } Mg(OH)_2} \text{ x } \frac{262.9\text{ g } Mg_3(PO_4)_2}{1\text{ mole } Mg_3(PO_4)_2}$$

= 20.9 g $Mg_3(PO_4)_2$

(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.

mass $Mg(OH)_2$ =

$$127 \text{ g } Mg_3(PO_4)_2 \times \frac{1 \text{ mole } Mg_3(PO_4)_2}{262.9 \text{ g } Mg_3(PO_4)_2} \times \frac{3 \text{ moles } Mg(OH)_2}{1 \text{ mole } Mg_3(PO_4)_2} \times \frac{58.3 \text{ g } Mg(OH)_2}{1 \text{ mole } Mg(OH)_2}$$

= 84.49 g $Mg(OH)_2$.

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

(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* $H_3PO_4$.

mass $Mg(OH)_2$ =

$$38.45 \text{ mL } H_3PO_4 \times \frac{0.6695 \text{ mole } H_3PO_4}{1000 \text{ mL } H_3PO_4} \times \frac{3 \text{ moles } Mg(OH)_2}{2 \text{ moles } H_3PO_4} \times \frac{58.3 \text{ g } Mg(OH)_2}{1 \text{ mole } Mg(OH)_2}$$

= 2.251 g $Mg(OH)_2$. Percent purity = $\frac{2.251}{2.568} \times 100 = 87.7\%$

Consider the reaction $4PH_3 + 8O_2 \rightarrow P_4O_{10} + 6H_2O$

(a) Calculate the theoretical yield of $P_4O_{10}$ from the reaction of 15.0 g of 88.0% $PH_3$ with excess $O_2$. (*Ans*. 27.6 g)

(b) What mass of 94.0% $PH_3$ is needed to make 500.0 g of $P_4O_{10}$, 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 $O_2$ to produce 39.3 g of $H_2O$. (*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%)

$$Al_2O_3(s) + 3H_2SO_4(aq) \rightarrow Al_2(SO_4)_3(aq) + 3H_2O(l)$$

## 4. LIMITING REACTANTS

(a) Consider the reaction $Ca_3N_2 + 6H_2O \rightarrow 2NH_3 + 3Ca(OH)_2$
For the reaction of 20.0 g of $Ca_3N_2$ with 16.0 g of $H_2O$,
(1) calculate the theoretical yield of $Ca(OH)_2$,
(2) determine the limiting reactant, and
(3) calculate the mass of the excess reactant left over.

*Solution*:

From $Ca_3N_2$: mass of $Ca(OH)_2$ = 20.0 g $Ca_3N_2$ x $\dfrac{3 \text{ x } 74.1 \text{ g } Ca(OH)_2}{148.3 \text{ g } Ca_3N_2}$ = 30.0 g

From $H_2O$: mass of $Ca(OH)_2$ = 16.0 g $H_2O$ x $\dfrac{3 \text{ x } 74.1 \text{ g } Ca(OH)_2}{6 \text{ x } 18.0 \text{ g } H_2O}$ = 32.9 g

(1) the theoretical yield of $Ca(OH)_2$ is 30.0 g.
(2) the limiting reactant is $Ca_3N_2$.
(3) the mass of $H_2O$ reacted = 20.0 g $Ca_3N_2$ x $\dfrac{6 \text{ x } 18.0 \text{ g } H_2O}{148.3 \text{ g } Ca_3N_2}$ = 14.6 g

mass of $H_2O$ left over = (16.0 - 14.6) g = 1.4 g

(b) For the reaction $4PH_3 + 8O_2 \rightarrow P_4O_{10} + 6H_2O$ calculate (1) the theoretical yield of $P_4O_{10}$, and (2) the mass of the excess reactant left over when 35.0 g of $PH_3$ were reacted with 60.0 g of $O_2$. [*Ans*. (1) 66.6 g $P_4O_{10}$, (2) 3.1 g $PH_3$]

(c) Consider the reaction $3NaBH_4 + 4BF_3 \rightarrow 3NaBF_4 + 2B_2H_6$
The reaction was carried out using 78.0 g of $NaBH_4$ and 172.0 g of $BF_3$. Calculate
(1) the theoretical yield of $B_2H_6$, and
(2) the mass of the excess reactant left over.
[*Ans*. (1) 35.0 g $B_2H_6$, (2) 6.1 g $NaBH_4$]

## 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 rigourous 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 ($CH_4$; the main constituent of natural gas). The equation for the reaction is given below.

$$CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(l) + 890\ \text{kJ}$$

An example of an endothermic reaction is the reaction of nitrogen with oxygen to produce $N_2O$. This reaction can be written

$$2N_2(g) + O_2(g) + 163\ \text{kJ} \rightarrow 2N_2O(g)$$

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 $CH_4(g)$ reacts with $O_2(g)$ to produce 1 mole of $CO_2(g)$ and 2 moles of $H_2O(l)$, 890 kJ of heat are released. [Note that the reaction of 1 mole of $CH_4(g)$ with $O_2(g)$ to produce 1 mole of $CO_2(g)$ and 2 moles of $H_2O(g)$ would produce less heat because heat is needed to convert $H_2O(l)$ (liquid water) to $H_2O(g)$ (water vapour)]. Hence, thermochemical equations can be treated as other equations for stoichiometric calculations.

***Example***

The reaction for the combustion of ethane gas ($C_2H_6$) is given below.

$$2C_2H_6(g) + 7O_2(g) \rightarrow 4\ CO_2(g) + 6H_2O(l) + 3119\ \text{kJ}$$

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

$$555\ \text{g}\ C_2H_6 \times \frac{1\ \text{mole}\ C_2H_6}{30.0\ \text{g}\ C_2H_6} \times \frac{3119\ \text{kJ}}{2\ \text{moles}\ C_2H_6} = 2.89 \times 10^4\ \text{kJ}$$

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

$$955\ \text{kJ} \times \frac{6\ \text{moles}\ H_2O}{3119\ \text{kJ}} \times \frac{18.0\ \text{g}\ H_2O}{1\ \text{mole}\ H_2O} = 33.1\ \text{g}\ H_2$$