STOICHIOMETRY – calculations using stoichiometric coefficients from balanced reactions

Example 1: How many grams NH₃(g) can be prepared from 84.0g N₂(g) in this reaction: N₂(g) + 3H₂(g) → 2NH₃(g)

Answer 1: This is a “grams A → grams B” calculation (see diagram above); it requires 3 conversions (the steps are shown in the flowchart)

Step 1: N₂ + 3H₂ → 2NH₃

Step 2: 3-step conversion: gA \( \frac{1 \text{ mol A}}{gA} \) \( \frac{1 \text{ mol B}}{1 \text{ mol A}} \) \( \frac{gB}{1 \text{ mol B}} \) = gB

Step 3: 3-step conversion: 84.0g N₂ \( \frac{1 \text{ mol N₂}}{28.0g N₂} \) \( \frac{2 \text{ mol NH₃}}{1 \text{ mol N₂}} \) \( \frac{17.0g NH₃}{1 \text{ mol NH₃}} \) = 102g NH₃

LIMITING REAGENTS: one reagent runs out first – this is the limiting reagent; a limiting reagent problem can be identified when 2 reactant quantities are given in the problem; many ways to solve these types of problems - one way: calculate the amount of products possible from each reactant quantity; the smaller amount produced is the theoretical amount that can be made; the reactant that gives this smaller amount is the limiting reagent

Example 2: a. How many grams Al₂O₃(s) can be made from 25.0g Al(s) and 20.0g O₂(g) using: 4Al(s) + 3O₂(g) → 2Al₂O₃(s)?

b. Which reactant is the limiting reagent?

c. Which reagent is the excess reagent?

d. How much of the excess reagent remains after the reaction is complete?

Answer 2: This is a limiting reagent problem since 2 reactant quantities were given in the problem. The amount produced can be solved by doing two “grams A → grams B” calculations, and then comparing the two possible amounts of Al₂O₃(s) produced. The amount of excess reagent left over will require a third “grams A → grams B” calculation requiring 3 steps.

\[
\begin{align*}
\text{Step 1: gA → gB calculation: } & 4 \text{ mol Al} \rightarrow 1 \text{ mol Al₂O₃} \\
& \frac{1 \text{ mol Al₂O₃}}{4 \text{ mol Al}} \times 25.0g \text{ Al} = 19.2g \text{ Al₂O₃} \\
\text{Step 2: gA → gB calculation: } & 3 \text{ mol O₂} \rightarrow 2 \text{ mol Al₂O₃} \\
& \frac{1 \text{ mol Al₂O₃}}{3 \text{ mol O₂}} \times 20.0g \text{ O₂} = 13.3g \text{ Al₂O₃} \\
\text{Step 3: gA → gB calculation: } & 2 \text{ mol Al} \rightarrow 2 \text{ mol Al₂O₃} \\
& \frac{1 \text{ mol Al₂O₃}}{2 \text{ mol Al}} \times 22.5g \text{ Al} = 22.5g \text{ Al₂O₃}
\end{align*}
\]

a. 42.5g Al₂O₃ \{the smaller quantity of Al₂O₃(s) is how much can theoretically be produced\}

b. O₂(g) is the LR \{since it produced the smaller amount Al₂O₃(s)\}

c. Al(s) is the excess reagent \{since it produced the larger amount Al₂O₃(s)\}

d. 2.5g Al left over \{Amount Excess Reagent Left Over = Starting Amount Excess Reagent – Used Amount Excess Reagent; \}

Used amount can be calculated with “grams A → grams B” with the calculation: LR → Excess reagent:

\[
\begin{align*}
\text{Step 3: gA → gB calculation: } & 2 \text{ mol Al} \rightarrow 2 \text{ mol Al₂O₃} \\
& \frac{1 \text{ mol Al₂O₃}}{2 \text{ mol Al}} \times 22.5g \text{ Al} = 22.5g \text{ Al used} \\
& 22.5g \text{ Al is the amount of the Excess Reagent used}
\end{align*}
\]

Amount Left Over = 25.0g Al – 22.5g Al = 2.5g Al left over}
PERCENT YIELD = \( \left( \frac{\text{actual yield}}{\text{theoretical yield}} \right) \times 100\% \)

Actual yield is the actual amount obtained and is always given in the problem; theoretical yield is usually calculated. In a lab setting, if the %yield > 100% then there is an error (e.g., the sample may be wet, etc.)

**EMPIRICAL FORMULA from mass CO₂ and H₂O (combustion reaction)**

A. Compound contains **C and H only**
   1. Convert gCO₂ \( \rightarrow \) mol CO₂ \( \rightarrow \) mol C
   2. Convert gH₂O \( \rightarrow \) mol H₂O \( \rightarrow \) mol H
   3. Write formula and divide by smallest moles
   4. If needed, fractions: \( \frac{1}{2} \) (0.5) \( \rightarrow \) x 2; \( \frac{1}{3} \) or \( \frac{2}{3} \) (0.33, 0.66) \( \rightarrow \) x 3; \( \frac{1}{4} \) or \( \frac{3}{4} \) (0.25, 0.75) \( \rightarrow \) x 4

B. Compound contains **C, H, and X** (used for a C, H, and X compound; X is a third element often O or N; example below has X = O)
   1. Convert gCO₂ \( \rightarrow \) mol CO₂ \( \rightarrow \) mol C; mol C \( \rightarrow \) gC (need both mol C and gC)
   2. Convert gH₂O \( \rightarrow \) mol H₂O \( \rightarrow \) mol H; mol H \( \rightarrow \) gH (need both mol H and gH)
   3. Calculate gO from: total g sample = gC + gH + gO (gO = total g sample - gC - gH)
   4. Convert gO \( \rightarrow \) mol O
   5. Write formula and divide by smallest moles
   6. If needed, fractions: \( \frac{1}{2} \) (0.5) \( \rightarrow \) x 2; \( \frac{1}{3} \) or \( \frac{2}{3} \) (0.33, 0.66) \( \rightarrow \) x 3; \( \frac{1}{4} \) or \( \frac{3}{4} \) (0.25, 0.75) \( \rightarrow \) x 4

**Example 3:** Butane, a hydrocarbon, was burned and 15.14g CO₂ and 7.751g H₂O are recovered. What is the empirical formula of butane?

**Answer 3:** C₂H₅

1. mol C: 15.14gCO₂ \( \left( \frac{1molCO₂}{44.01gCO₂} \right) \left( \frac{1molC}{1molCO₂} \right) = 0.3441molC \)
2. mol H: 7.751gH₂O \( \left( \frac{1molH₂O}{18.02gH₂O} \right) \left( \frac{2molH}{1molH₂O} \right) = 0.8603molH \)
3. Write formula: C\(_{0.3441}\)H\(_{0.8603}\) and divide by smallest number of mol = 0.3441: C\(_{\frac{0.3441}{0.3441}}\)H\(_{\frac{0.8603}{0.3441}}\) \( \rightarrow \) empirical formula = C\(_2\)H\(_5\)

**Example 4:** When 2.000g of a compound containing carbon, hydrogen, and oxygen is combusted, 1.912g CO₂ and 0.7830g H₂O are recovered. What is the empirical formula?

**Answer 4:** CH₂O₂

1. mol C: 1.912gCO₂ \( \left( \frac{1molCO₂}{44.01gCO₂} \right) \left( \frac{1molC}{1molCO₂} \right) = 0.04344molC and gC: 0.04344molC \( \left( \frac{12.01gC}{1molC} \right) = 0.5217gC \)
2. mol H: 0.7830gH₂O \( \left( \frac{1molH₂O}{18.02gH₂O} \right) \left( \frac{2molH}{1molH₂O} \right) = 0.08690molH and gH: 0.08690molH \( \left( \frac{1.008gH}{1molH} \right) = 0.08760gH \)
3. gO: \( g_{\text{sample}} = gC + gC + gH \) \( \rightarrow \) solve for \( gO \): \( gO = g_{\text{sample}} - gC - gH = 2.000 - 0.5217 - 0.08760 = 1.3907gO \)
4. mol O: 1.3907gO \( \left( \frac{1molO}{16.00gO} \right) = 0.08692molO \)
5. Write formula: C\(_{0.04344}\)H\(_{0.08690}\)O\(_{0.08692}\); divide by smallest number of mol = 0.04344: C\(_{\frac{0.04344}{0.04344}}\)H\(_{\frac{0.08690}{0.04344}}\)O\(_{\frac{0.08692}{0.04344}}\) = C\(_1\)H\(_2\)O\(_2\)
6. Fractions: no fractions; this step not needed

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1. Nitric acid, HNO₃, is manufactured by the Oswald process, in which nitrogen dioxide, NO₂, reacts with H₂O. How many grams of NO₂ are required to produce 5.00g HNO₃.

\[ 3\text{NO}_2(g) + \text{H}_2\text{O}(l) \rightarrow 2\text{HNO}_3(aq) + \text{NO}(g) \]

a. 7.50  
   b. 15.0  
   c. 3.65  
   d. 0.120  
   e. 5.48
2. Calculate the masses (in grams) of Cr$_2$O$_3$ (chromium(III) oxide), N$_2$, and H$_2$O produced from 10.8g of (NH$_4$)$_2$CrO$_7$ (ammonium dichromate) in the following balanced reaction:

$$(\text{NH}_4)_2\text{Cr}_2\text{O}_7(s) \rightarrow \text{Cr}_2\text{O}_3(s) + \text{N}_2(g) + 4\text{H}_2\text{O(l)}$$

3. a. When 9.20g of C$_2$H$_6$O are reacted with 40.6g of PBr$_3$, what mass of C$_2$H$_5$Br can be produced?

$$3\text{C}_2\text{H}_6\text{O} + \text{PBr}_3 \rightarrow 3\text{C}_2\text{H}_5\text{Br} + \text{H}_3\text{PO}_3$$

b. Which reactant is the limiting reagent?
c. Which reactant is the excess reagent?
d. How much of the excess reagent is left over?
e. If 10.9g PBr$_3$ was recovered after the experiment, what was the %yield of this reaction?

4. If 75.0g of SiO$_2$ and 30.0g C react according to the equation below, what is the maximum number of moles of CO that can be produced?  

$$\text{SiO}_2 + \text{C} \rightarrow \text{CO} + \text{SiO}$$
a. 1.25  
b. 1.67  
c. 2.25  
d. 2.50  
e. none of these

5. I. Given the following balanced combustion reaction below, if there were 3.0mol of C$_2$H$_4$ and 6.0mol of O$_2$, how many moles of CO$_2$ could theoretically be produced?

$$\text{C}_2\text{H}_4 + 3\text{O}_2 \rightarrow 2\text{CO}_2 + 2\text{H}_2\text{O}$$
a. 6mol  
b. 4mol  
c. 9mol  
d. 3mol  
e. 7mol

II. After the above reaction was completed, 3.5mol of CO$_2$ were actually obtained. What is the percent yield of this reaction? (Note: You can only do this part with the correct answer to part I.)

6. Consider the reaction:

$$2\text{H}_2(\text{g}) + \text{O}_2(\text{g}) \rightarrow 2\text{H}_2\text{O}(\text{g})$$

Identify the limiting reagent in each of the reaction mixtures below. Note: This is not a multiple choice question.

a. 0.50mol of H$_2$ and 0.75mol of O$_2$  
b. 0.80mol of H$_2$ and 0.75mol of O$_2$  
c. 1.00g of H$_2$ and 0.35mol of O$_2$  
d. 5.00g of H$_2$ and 64.00g of O$_2$

7. When a compound containing carbon and hydrogen is combusted, 3.38g CO$_2$ and 0.692g H$_2$O are recovered. 
a. What is the empirical formula?  
b. The molar mass of the compound is 78.1g/mol. What is the molecular formula?

8. When 5.000g of a compound containing carbon, hydrogen, and oxygen is combusted, 8.910g CO$_2$ and 3.648g H$_2$O are recovered. 
a. What is the empirical formula?  
b. The molar mass of the compound is 74.1g/mol. What is the molecular formula?

9. A compound contains carbon, hydrogen, and nitrogen. When 0.9731 gram of this substance is combusted, 2.3744grams CO$_2$ and 1.2153grams of H$_2$O are collected. What is the empirical formula?

**ANSWERS**

1. e  
   \{ 5.00g HNO$_3$ \left(\frac{1\text{mol HNO}_3}{63.02g \text{HNO}_3}\right) \left(\frac{3\text{mol NO}_2}{2\text{mol HNO}_3}\right) \left(\frac{46.01g \text{NO}_2}{1\text{mol NO}_2}\right) = 5.476g \text{ NO}_2 \}
2. 6.52g Cr$_2$O$_3$ \{10.8g (NH$_4$)$_2$Cr$_2$O$_7$ \left( \frac{1mol \text{ (NH}_4\text{)}_2\text{Cr}_2\text{O}_7}{252.08g \text{ (NH}_4\text{)}_2\text{Cr}_2\text{O}_7} \right) \left( \frac{1mol \text{ Cr}_2\text{O}_3}{1mol \text{ (NH}_4\text{)}_2\text{Cr}_2\text{O}_7} \right) \left( \frac{152.00g \text{ Cr}_2\text{O}_3}{1mol \text{ Cr}_2\text{O}_3} \right) \} \approx 65.12g \text{ Cr}_2\text{O}_3\}

1.20g N$_2$ \{10.8g (NH$_4$)$_2$Cr$_2$O$_7$ \left( \frac{1mol \text{ (NH}_4\text{)}_2\text{Cr}_2\text{O}_7}{252.08g \text{ (NH}_4\text{)}_2\text{Cr}_2\text{O}_7} \right) \left( \frac{1mol \text{ N}_2}{1mol \text{ (NH}_4\text{)}_2\text{Cr}_2\text{O}_7} \right) \left( \frac{28.02g \text{ N}_2}{1mol \text{ N}_2} \right) \} \approx 1.200g \text{ N}_2\}

3. 0.09g H$_2$O \{10.8g (NH$_4$)$_2$Cr$_2$O$_7$ \left( \frac{1mol \text{ (NH}_4\text{)}_2\text{Cr}_2\text{O}_7}{252.08g \text{ (NH}_4\text{)}_2\text{Cr}_2\text{O}_7} \right) \left( \frac{4mol \text{ H}_2\text{O}}{1mol \text{ (NH}_4\text{)}_2\text{Cr}_2\text{O}_7} \right) \left( \frac{18.02g \text{ H}_2\text{O}}{1mol \text{ H}_2\text{O}} \right) \} \approx 3.088g \text{ H}_2\text{O}\}

3. a. 21.8g C$_2$H$_5$Br \{limiting reagent problem since 2 reactant quantities are given;

b. C$_2$H$_6$O is LR \{the chemical that produced the smaller amount of C$_2$H$_5$Br\}

c. PBr$_3$ is the excess reagent \{the chemical that produced the larger amount of C$_2$H$_5$Br\}

d. 22.6g PBr$_3$ \{Left over = starting amount – amount used; amount used = g A \rightarrow g B going from LR \rightarrow Excess Reagent;\}

\[
9.20g \text{ C}_2\text{H}_6\text{O} \left( \frac{1mol \text{ C}_2\text{H}_6\text{O}}{46.07g \text{ C}_2\text{H}_6\text{O}} \right) \left( \frac{3mol \text{ C}_2\text{H}_5\text{Br}}{3mol \text{ C}_2\text{H}_6\text{O}} \right) \left( \frac{108.96g \text{ C}_2\text{H}_5\text{Br}}{1mol \text{ C}_2\text{H}_5\text{Br}} \right) = 21.76g \text{ C}_2\text{H}_5\text{Br} ;
\]

\[
40.6g \text{ PBr}_3 \left( \frac{1mol \text{ PBr}_3}{270.67g \text{ PBr}_3} \right) \left( \frac{3mol \text{ C}_2\text{H}_5\text{Br}}{3mol \text{ C}_2\text{H}_6\text{O}} \right) \left( \frac{108.96g \text{ C}_2\text{H}_5\text{Br}}{1mol \text{ C}_2\text{H}_5\text{Br}} \right) = 49.03g \text{ C}_2\text{H}_5\text{Br} ;
\]

the smaller amount of C$_2$H$_5$Br is the theoretical yield that can be produced\}

e. 50.0\% \{\% yield = (actual yield/theoretical yield) \times 100\%; \% yield = (10.9g C$_2$H$_5$Br/21.8g C$_2$H$_5$Br) \times 100\% \approx 50.0\%\}

4. a. \{limiting reagent problem since 2 reactant quantities are given;\}

\[
75.0g \text{ SiO}_2 \left( \frac{1mol \text{ SiO}_2}{60.09g \text{ SiO}_2} \right) \left( \frac{1mol \text{ CO}}{1mol \text{ SiO}_2} \right) = 1.248mol \text{ CO} ;
\]

30.0g C \left( \frac{1mol \text{ C}}{12.01g \text{ C}} \right) \left( \frac{1mol \text{ CO}}{1mol \text{ C}} \right) = 2.498mol \text{ CO} ;
\]

the smaller amount of CO is the theoretical yield\}

5. I. b. \{limiting reagent problem; \{3mol C$_2$H$_4$ \left( \frac{2mol \text{ CO}_2}{1mol \text{ C}_2\text{H}_4} \right) = 6mol \text{ CO}_2; \{6mol O$_2$ \left( \frac{2mol \text{ CO}_2}{3mol \text{ O}_2} \right) = 4mol \text{ CO}_2;\}

choose smaller amount \rightarrow 4mol \text{ CO}_2\}

II. 87.5\% \{\% yield = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100\%; \% yield = \frac{3.5mol \text{ CO}_2}{4.0mol \text{ CO}_2} \times 100\% \approx 87.5\%\}

6. a. H$_2$  b. H$_2$  c. O$_2$  d. H$_2$

7. a. CH \{3.38g CO \left( \frac{1mol \text{ CO}_2}{44.01g \text{ CO}_2} \right) \left( \frac{1mol \text{ C}}{1mol \text{ CO}_2} \right) = 0.0768mol \text{ C}; 0.692g H$_2$O \left( \frac{1mol \text{ H}_2\text{O}}{18.02g \text{ H}_2\text{O}} \right) \left( \frac{2mol \text{ H}}{1mol \text{ H}_2\text{O}} \right) = 0.0768mol \text{ H};\}

write formula: C$_{0.07680}$H$_{0.07680}$O$_{0.07680}$; divide by 0.07680: C$_{0.07680}$/H$_{0.07680}$/O$_{0.07680}$ \rightarrow C$_1$H$_1$ = EF\}

b. C$_6$H$_6$ \{ratio = \frac{\text{molar mass}_{\text{molecular formula}}}{\text{molar mass}_{\text{empirical formula}}} = \frac{78.1}{13.02} \approx 5.998 = 6; multiply EF by 6; C(1 \times 6)H(1 \times 6) = C_6H_6 = \text{MF}\}
8. a. \( C_3H_6O_2 \quad \{ 8.910g \text{ CO}_2 \left( \frac{1 \text{ mol CO}_2}{44.01g \text{ CO}_2} \right) \left( \frac{1 \text{ mol C}}{1 \text{ mol CO}_2} \right) = 0.2025 \text{ mol C} ; \ gC = 0.2025 \text{ mol C} \times (12.01g \text{ C}/1 \text{ mol C}) = 2.4320g \text{ C} ; \}

\[
3.648g \text{ H}_2O \left( \frac{1 \text{ mol H}_2O}{18.02g \text{ H}_2O} \right) \left( \frac{2 \text{ mol H}}{1 \text{ mol H}_2O} \right) = 0.4049 \text{ mol H} ; \ gH = 0.4049 \text{ mol H} \times (1.008g \text{ H}/1 \text{ mol H}) = 0.4081g \text{ H} ;
\]

\( g_{\text{sample}} = gO + gC + gH \rightarrow \text{ solve for } gO: \ gO = g_{\text{sample}} - gC - gH = 5.00 - 2.4320 - 0.4081 = 2.1599g \text{ O} \)

\[
2.1599g \text{ O} \left( \frac{1 \text{ mol O}}{16.00g \text{ O}} \right) = 0.1350 \text{ mol O} ;
\]

\( C_{0.2025}H_{0.4049}O_{0.1350} ; \ \text{ divide by 0.1350: } C_{0.2025} \times \frac{H_{0.4049}}{0.1350} \times \frac{O_{0.1350}}{0.1350} = C_{1.500}H_{2.999}O_{1} ; \ \text{ fraction of 0.5 } \rightarrow \frac{1}{2} \rightarrow x2: C_{(1.500}}^\text{H}_{(2.999 \times 2)}O_{(1 \times 2)} = C_3H_5O_2 = \text{ EF} \}

b. \( C_3H_6O_2 \quad \{ \text{ ratio } = \frac{\text{ molar mass}}{\text{ molecular formula}} \frac{\text{ molar mass}}{\text{ empirical formula}} = \frac{74.1}{74.08} = 1.000 ; \ \text{ multiply EF by 1; } C_{(3 \times 1)}H_{(6 \times 1)}O_{(2 \times 1)} = C_3H_6O_2 = \text{ MF} \}

9. \( C_4H_{10}N \quad \{ 2.3744g \text{ CO}_2 \left( \frac{1 \text{ mol CO}_2}{44.01g \text{ CO}_2} \right) \left( \frac{1 \text{ mol C}}{1 \text{ mol CO}_2} \right) = 0.053951 \text{ mol C} ; \ gC = 0.053951 \text{ mol C} \times \left( \frac{12.01g \text{ C}}{1 \text{ mol C}} \right) = 0.64795g \text{ C} ; \}

\[
1.2153g \text{ H}_2O \left( \frac{1 \text{ mol H}_2O}{18.02g \text{ H}_2O} \right) \left( \frac{2 \text{ mol H}}{1 \text{ mol H}_2O} \right) = 0.13488 \text{ mol H} ; \ gH = 0.13488 \text{ mol H} \times \left( \frac{1.008g \text{ H}}{1 \text{ mol H}} \right) = 0.13596g \text{ H} ;
\]

\( g_{\text{sample}} = gN + gC + gH \rightarrow \text{ solve for } gN: \ gN = g_{\text{sample}} - gC - gH = 0.9731 - 0.64795 - 0.13596 = 0.18919g \text{ N} \)

\[
\text{ mol N} = 0.18919g \text{ N} \left( \frac{1 \text{ mol N}}{14.01g \text{ N}} \right) = 0.013504 \text{ mol N} ; \ C_{0.053951}H_{0.13488}N_{0.013504} ; \ \text{ divide by 0.013504: } C_{\frac{0.053951}{0.013504}}H_{\frac{0.13488}{0.013504}}N_{\frac{0.013504}{0.013504}} = C_{3.9952}H_{9.9882}N_{1} = C_4H_{10}N_1 = \text{ EF} \}