

CHEMICAL CALCULATIONS

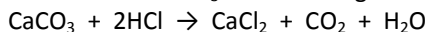
1. Simple Stoichiometric Calculations

- Calculations in which chemical equations and the coefficients are used to calculate the amount of one substance from a second substance are called stoichiometric calculations.
- “Stoichio” + “metry” means element + measure in Greek language.

$$\text{Remember that; } N_A = 6.02 \times 10^{23} \quad n = \frac{m}{M} = \frac{V}{22.4} = \frac{N}{N_A}$$

Example 1

When HCl is added to CaCO₃ the following reaction takes place;



How many grams of CaCO₃ should be reacted to obtain 4.214x10²² CO₂ molecules? (Ca: 40, C: 12, O: 16)

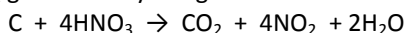
Solution

$$n_{\text{CO}_2} = \frac{4.214 \times 10^{22}}{6.02 \times 10^{23}} = 0.07 \text{ mol}$$

1 mol of CO₂ is produced from 1 mol CaCO₃
0.07 mol of CO₂ is produced from x mol CaCO₃
x = 0.07 mol CaCO₃
M_{CaCO₃} = 40 + 12 + 3x16 = 100 g/mol
m_{CaCO₃} = nxM = 0.07x100 = 7 g mass of CaCO₃

Example 2

How many grams of C must be reacted in order to produce 4.48 L of NO₂ gas at STP by the given reaction below? (C: 12)



Solution

$$n_{\text{NO}_2} = \frac{4.48}{22.4} = 0.2 \text{ mol}$$

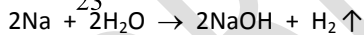
4 mol of NO₂ is produced from 1 mol C
0.2 mol of NO₂ is produced from x mol C
x = 0.05 mol C
m_C = nxM = 0.05x12 = 0.6 g mass of C

Example 3

How many liters of H₂ gas at STP is evolved when 2.3 g of Na is put in enough water? (Na: 23)

Solution

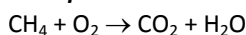
$$n_{\text{Na}} = \frac{2.3}{23} = 0.1 \text{ mol}$$



2 mol of Na produces 1 mol H₂
0.1 mol of Na produces x mol H₂
x = 0.05 mol H₂

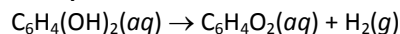
$$V_{\text{H}_2} = nx22.4 = 0.05 \times 22.4 = 1.12 \text{ L of H}_2$$

Example 4



A sample of methane, CH₄, was burned in air at STP and the above reaction occurred. If 112 liters of CO₂ were produced and all of the carbon in the CO₂ came from the methane, what was the mass of the methane sample?

Example 5



According to the equation above, if 224 liters of H₂ gas was found to be produced at standard temperature and pressure, what amount (in grams) of C₆H₄(OH)₂(aq) solution was there initially?

2. Limiting Reagent Problems

- Rarely are the reactants in a chemical reaction present in the exact mole ratios specified in the balanced equation.
- Usually, one or more of the reactants are present in excess, and the reaction proceeds until all of one reactant is used up.
- The reactant that is used up is called the limiting reactant.
- The limiting reactant limits the reaction and, thus, determines how much of the product forms.
- The left-over reactants are called excess reactants.

Example 6

By using 8 grams for each of Ca and Br₂, how many grams of CaBr₂ is possible to be produced? (Ca: 40, Br: 80)

Solution

$$n_{\text{Ca}} = \frac{8}{40} = 0.2 \text{ mol}$$

$$n_{\text{Br}_2} = \frac{8}{160} = 0.05 \text{ mol}$$

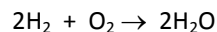
$$M_{\text{CaBr}_2} = 40 + 2 \times 80 = 200 \text{ g/mol}$$

$$m_{\text{CaBr}_2} = nxM = 0.05 \times 200 = 10 \text{ g}$$

	Ca	+ Br ₂	→	CaBr ₂
Initial:	0.2 mol	0.05 mol		-
Change:	-0.05	-0.05		+0.05
Final:	0.15 mol	0 mol		0.05 mol
	(Excess)	(Limiting)		

Example 7

96 grams for each of the gases H₂ and O₂ are burnt with a spark as follow;



- How many grams of water is formed?
- Which one is the excess reactant and how many grams of it will remain unreacted? (H: 1, O: 16)

$$n_{\text{H}_2} = \frac{96}{2} = 48 \text{ mol}$$

$$n_{\text{O}_2} = \frac{96}{32} = 3 \text{ mol}$$

	2H ₂	+ O ₂	→	2H ₂ O
Initial:	48 mol	3 mol		-
Change:	-6	-3		+6
Final:	42 mol	0 mol		6 mol
	(Excess)	(Limiting)		

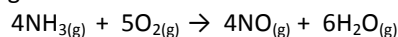
$$M_{\text{H}_2\text{O}} = 2 \times 1 + 16 = 18 \text{ g/mol}$$

a.
m_{H₂O} = nxM = 6x18 = 108 g of H₂O

b.
m_{H₂ Excess} = nxM = 42x2 = 84 g of H₂

Example 8

A 17 g sample of ammonia is mixed with 16 g of oxygen, according to the reaction below.



Which is the limiting reactant and how much excess reactant remains after the reaction has stopped?

3. Percent Yield

$$\text{Percent Yield} = \frac{\text{Practical Amount}}{\text{Theoretical Amount}} \cdot 100$$

$$\text{Yield} = \frac{n_{\text{practical}}}{n_{\text{theoretical}}} \quad \text{Yield} = \frac{V_{\text{practical}}}{V_{\text{theoretical}}} \quad \text{Yield} = \frac{m_{\text{practical}}}{m_{\text{theoretical}}}$$

Example 9

What is the percent yield for a reaction if you predicted the formation of 21 grams of C_6H_{12} and actually recovered only 3.8 grams?

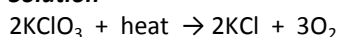
Solution

$$\% \text{ Yield} = \frac{3.8 \text{ g}}{21 \text{ g}} \times 100 = 18\%$$

Example 10

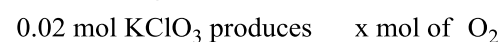
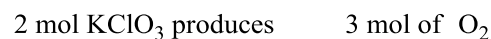
O_2 gas is obtained from the decomposition of $KClO_3$ by heating. 0.8 g of O_2 gas is obtained from 2.45 g of $KClO_3$. What is the percent yield of this reaction? (K: 39, Cl:35.5, O: 16)

Solution



$$M_{KClO_3} = 39 + 35.5 + 3 \times 16 = 122.5 \text{ g/mol}$$

$$M_{O_2} = 2 \times 16 = 32 \text{ g/mol}$$



$$x = \frac{3 \times 0.02}{2} = 0.03 \text{ mol } O_2$$

$$n_{KClO_3} = \frac{2.45}{122.5} = 0.02 \text{ mol}$$

$$n_{O_2} = \frac{0.8}{32} = 0.025 \text{ mol}$$

$$\% \text{ Yield} = \frac{n_{\text{practical } O_2}}{n_{\text{theoretical } O_2}} \times 100 = \frac{0.025}{0.03} \times 100 = 83$$

Example 11

A reaction between solid sulfur and oxygen produces sulfur dioxide.

The reaction started with 384 grams of S_8 (s). Assume an unlimited supply of oxygen. What is the predicted yield and the percent yield if only 680 grams of sulfur dioxide are produced? (S:32, O:16)

Example 12

What is the % yield of H_2O if 58 g H_2O are produced by combining 60 g O_2 and 7.0 g H_2 ?

4. Determination of Unknown Substances

Formula which gives type and ratio of combining elements in a compound is called empirical or simplest formula.

Formula which gives type, ratio and exact number of combining elements in a compound is called molecular or real formula.

$$x = \frac{M_{\text{molecular Formula}}}{M_{\text{empirical Formula}}}$$

Substance	Empirical Formula	X	Molecular Formula
Benzene	CH	6	C_6H_6
Phosphorus	P	4	P_4
Glucose	CH_2O	6	$C_6H_{12}O_6$

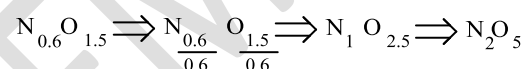
Example 13

0.3 moles of a compound containing nitrogen and oxygen is produced after the reaction of 19.2 grams of oxygen and 6.72 liters of N_2O at STP. What is the empirical formula of this compound? (N: 14, O: 16)

Solution

$$n_{N_2O} = \frac{6.72}{22.4} = 0.3 \text{ mol} \quad n_N = 0.3 \times 2 = 0.6 \text{ mol} = x$$

$$n_{O_2} = \frac{19.2}{32} = 0.6 \text{ mol} \quad n_O = 2 \times 0.6 + 0.3 \text{ (from } N_2O) = 1.5 \text{ mol} = y$$



Example 14

Lactic acid is composed of C-H-O atoms and has a molar mass of 90 g/mol. 25.2 g of a sample of lactic acid contains 10.08 g of C and 13.44 g of oxygen. What is the molecular formula of lactic acid? (C: 12, H: 1, O: 16)

$$m_H = 25.2 - (m_C + m_O) = 25.2 - (10.08 + 13.44) = 1.68 \text{ g}$$

$$n_C = \frac{10.08}{12} = 0.84 \text{ mol}$$

$$n_H = \frac{1.68}{1} = 1.68 \text{ mol}$$

$$n_O = \frac{13.44}{16} = 0.84 \text{ mol}$$

$$C_{0.84}H_{1.68}O_{0.84}$$



$$M_{\text{empirical formula}} = 1 \times 12 + 2 \times 1 + 1 \times 16 = 30 \text{ g/mol}$$

$$M_{\text{empirical formula}} \cdot X = M_{\text{molecular formula}}$$

$$30 \cdot X = 90 \rightarrow X = 3 \text{ then } (CH_2O)_3 = C_3H_6O_3$$

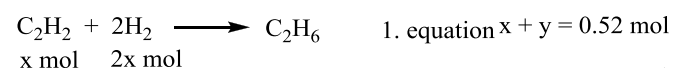
5. Mixture Problem

- In solving mixture problems,
 - check if all components react with that reagent or not,
 - write equations for all possible reactions,
 - find the desired quantity by the given equations.

Example 15

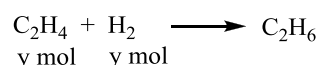
0.52 moles of C_2H_2 and C_2H_4 mixture was reacted with 0.7 mol H_2 gas. As a result of the reaction, all the gases are turned into C_2H_6 . What are the mole numbers for each gas in the mixture?

Solution



$$x \text{ mol} \quad 2x \text{ mol}$$

$$2x + y = 0.7 \text{ mol}$$



$$y \text{ mol} \quad y \text{ mol}$$

$$2. \text{ equation } x = 0.18 \text{ mol then}$$

$$0.18 + y = 0.52 \quad n_{\text{C}_2\text{H}_2} = 0.18 \text{ mol}$$

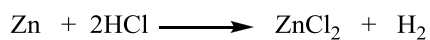
$$y = 0.34 \text{ mol} \quad n_{\text{C}_2\text{H}_4} = 0.34 \text{ mol}$$

Example 16

When a 10 g of Cu-Zn alloy is put in HCl solution, 2.24 L of H₂ gas is collected at STP. What is the mass of Cu in the alloy?

(Remember only Zn reacts in the alloy) (Zn: 65)

Solution Cu + HCl \longrightarrow No reaction



1 mol Zn produces 1 mol H₂

$$n = \frac{2.24}{22.4} = 0.1 \text{ mol}$$

x mol Zn produces 0.1 mol H₂

$$x = 0.1 \text{ mol Zn}$$

$$m_{\text{Zn}} = n \times M = 0.1 \times 65 = 6.5 \text{ g then}$$

$$m_{\text{Cu}} = 10 - m_{\text{Zn}} = 10 - 6.5 = 3.5 \text{ g}$$