

Basic Mathematics

Chemistry

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The aim of this document is to provide a short, self assessment programme for students who wish to apply some mathematical techniques to chemical applications.

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Table of Contents

1. Moles and Masses
 2. Density
 3. Concentrations of Chemicals in Solution
 4. Thermodynamics
 5. Kinetics
- Solutions to Exercises
- Solutions to Quizzes

1. Moles and Masses

The number of **moles** of a substance is defined as

$$\text{number of moles} = \frac{\text{mass}}{RMM}$$

where the mass is in grammes (denoted by **g**) and **RMM** denotes the **Relative Molecular Mass** of the substance.

Example 1 Calculate the number of moles of sodium chloride (**NaCl**) in 5.85 **g** given the **Relative Atomic Mass** data **Na**=23, **Cl**=35.5.

Solution From the question, the **RAMs** for **Na** and **Cl** are, respectively, 23 and 35.5. The **RMM** for **NaCl** is thus $23 + 35.5 = 58.5$. The number of moles is thus

$$\text{number of moles} = \frac{\text{mass}}{RMM} = \frac{5.85}{58.5} = 0.1.$$

EXERCISE 1. Given the following additional RAM data: Mg=24, C=12, H=1, calculate the following.

(Click on green letters for solutions.)

- (a) The number of moles in 0.95 g of magnesium chloride (MgCl_2).
- (b) The mass of 0.05 moles of Cl_2 .
- (c) The mass of 0.35 moles of benzene (C_6H_6).

Now try this quiz.

Quiz Given that the RAMs for S and O are 32 and 16 respectively, which of the following is the mass of 0.125 moles of MgSO_4 ?

- (a) 15 g,
- (b) 36 g,
- (c) 960 g,
- (d) 1.04×100^{-3} g.

2. Density

The **density** of a substance is defined to be its mass per unit of volume. Symbolically

$$\text{density} = \frac{\text{mass}}{\text{volume}}.$$

To see how this is used look at the following example.

Example 2 Find the **density** of water if 20 cm^3 has a mass of 20.4 g .

Solution Using the definition above,

$$\text{density} = \frac{\text{mass}}{\text{volume}} = \frac{20.4}{20} = 1.02 \text{ g cm}^{-3}.$$

On the next page are some exercises and a short quiz for practice.

EXERCISE 2. Use the formula for the **density** of a substance to calculate the following. (Click on **green** letters for solutions.)

- (a) The **volume** of 5 g of ethanol if its **density** is 0.8 g cm^{-3} .
- (b) The **mass** of 25 cm^3 of mercury if its **density** is 13.5 g cm^{-3}
- (c) The volume of 0.1 **moles** of acetone ($\text{C}_3\text{H}_6\text{O}$) if its **density** is 0.83 g cm^{-3} .

Now try this short quiz.

Quiz If the **density** of cyclohexane (C_6H_{12}) is 0.78 g cm^{-3} , which of the following is the number of **moles** in 100 cm^3 of the substance?

- (a) 1.53, (b) 0.66, (c) 1.08, (d) 0.93.

3. Concentrations of Chemicals in Solution

The **number of moles** of a chemical substance contained in a solution is defined by

$$\text{number of moles} = \frac{\text{volume} \times \text{molarity}}{1000}.$$

In this expression, the concentration term is represented by **molarity**. This can also be represented by **M** and is equivalent to the number of **moles** of substance in 1000 cm^3 , or 1 dm^3 , so the units are also in mol dm^{-3} .

Example 3 Calculate the **number of moles** of Cu^{2+} ions in 25 cm^3 of a 0.1 M solution.

Solution Using the definition above, we have

$$\text{number of moles} = \frac{\text{volume} \times \text{molarity}}{1000} = \frac{25 \times 0.1}{1000} = 2.5 \times 10^{-3}.$$

EXERCISE 3. Calculate the following. (Click on the green letters for solutions.)

- (a) A solution of Cl^- ions (0.35 M) was titrated and found to contain 7×10^{-4} moles of chloride. What volume was titrated?
- (b) An acidic solution (50 cm^3) is titrated and found to contain 5×10^{-2} moles of H^+ . What is the molarity of H^+ ?
- (c) Given that the pH of a substance is *minus* the \log_{10} of its molarity, what is the pH of the solution in part (b)?

And now a quiz.

Quiz If 11.1 g of CaCl_2 , with a Relative Molecular Mass of 111 g mol^{-1} is dissolved in 2500 cm^3 of water, which of the following pair represents the concentrations of Ca^{2+} and Cl^- ions?

- (a) 0.04 and 0.04 M, (b) 0.04 and 0.08 M,
(c) 0.25 and 0.05 M, (d) 4 and 8 M.

4. Thermodynamics

The **Gibbs** free energy equation is defined as

$$\Delta G = \Delta H - T\Delta S \quad (1)$$

where ΔG , ΔH , ΔS , correspond to the **Gibbs** free energy, the **enthalpy** and the **entropy** changes associated with a chemical process.

Example 4 Rearrange the above equation to give the equation in terms of the **enthalpy**, ΔH .

Solution Adding $T\Delta S$ to both sides of (1), we obtain

$$\Delta G + T\Delta S = \Delta H .$$

EXERCISE 4. Calculate the following. (Click on **green** letter for the solution.)

(a) Rearrange (1) to obtain ΔS as the subject of the equation.

EXERCISE 5. The standard equilibrium isotherm is defined as

$$\Delta G^0 = -RT \ln K, \quad (2)$$

where K corresponds to the equilibrium constant for a chemical reaction, and the superscript 0 denotes the isotherm.

- (a) Rearrange (2) to obtain an expression for $\ln K$.
(b) Given that $\ln 10 \simeq 2.3$, determine the expression for the equilibrium isotherm in terms of $\log_{10} K$.

Now there is a short quiz.

Quiz Combining (1) and (2), one can generate a further equation, known as the *van't Hoff* equation, which relates $\ln K$ to ΔH , ΔS and T . Which of those below is this equation?

- (a) $\ln K = \frac{\Delta H^0}{RT} - \frac{\Delta S^0}{R}$, (b) $\ln K = \Delta H^0 - T\Delta S^0 + RT$,
(c) $\ln K = -\frac{\Delta H^0}{RT} + \frac{\Delta S^0}{R}$, (d) $\ln K = RT - \Delta H^0 - T\Delta S^0$.

5. Kinetics

When two chemical species, **A** and **B**, with concentrations $[A]$ and $[B]$ respectively, react together, the general rate equation for the reaction is

$$\text{Rate} = k[A]^x[B]^y, \tag{3}$$

where k is the rate constant and x and y are the appropriate stoichiometric coefficients.

Quiz Using (3), which of the following is true when $x = 0$?

- (a) $\text{Rate} = 0$, (b) $\text{Rate} = k$,
(c) $\text{Rate} = k[B]^y$, (d) $\text{Rate} = \infty$.

Quiz Which of the following is an alternative expression?

- (a) $\log \text{Rate} = \log k[A][B]xy$,
(b) $\log \text{Rate} = \log k + [A] + x + [B] + y$,
(c) $\log \text{Rate} = \log k + x[A] + y[B]$,
(d) $\log \text{Rate} = \log k + x \log[A] + y \log[B]$.

The **Arrhenius** equation relates the rate constant, k , for a reaction to the **activation** energy E_a and the temperature, T , in Kelvin. It is

$$k = A \exp\left(-\frac{E_a}{RT}\right), \quad (4)$$

where R is the universal gas constant.

Quiz Which of the following is an alternative form of (4)?

- (a) $\ln k = \ln A - \frac{E_a}{RT}$, (b) $\ln k = \ln A - E_a - RT$,
(c) $\ln k = \ln A - E_a + RT$, (d) $\ln k = \ln A \left(\frac{-E_a}{RT}\right)$.

Quiz Which of the following also represents the **Arrhenius** equation?

- (a) $E_a = \ln(k/A)RT$, (b) $E_a = \frac{\ln(A/k)}{RT}$,
(c) $E_a = \frac{\ln(A/k)}{RT}$, (d) $E_a = \ln(A/k)RT$.

Solutions to Exercises

Exercise 1(a)

Since the RAMs for Mg and Cl are, respectively, 24 and 35.5, the RMM for MgCl_2 is

$$24 + (2 \times 35.5) = 24 + 71 = 95.$$

Then

$$\text{number of moles} = \frac{\text{mass}}{\text{RMM}} = \frac{0.95}{95} = 0.01.$$

Click on green square to return



Exercise 1(b)

The **RMM** for Cl_2 is $2 \times 35.5 = 71$. Rearranging the equation

$$\text{number of moles} = \frac{\text{mass}}{\text{RMM}}$$

we obtain

$$\begin{aligned} \text{mass} &= \text{number of moles} \times \text{RMM} \\ &= 0.05 \times 71 \\ &= 3.55 \text{ g.} \end{aligned}$$

Click on green square to return



Exercise 1(c)

The **RMM** for C_6H_6 is

$$(6 \times 12) + (6 \times 1) = 78.$$

Thus

$$\begin{aligned} \text{mass} &= \text{number of moles} \times \text{RMM} \\ &= 0.35 \times 78 \\ &= 27.3 \text{ g}. \end{aligned}$$

Click on green square to return



Exercise 2(a)

Since $\text{density} = \frac{\text{mass}}{\text{volume}}$,

a rearrangement of the equation gives

$$\text{volume} = \frac{\text{mass}}{\text{density}} = \frac{5}{0.8} = 6.25 \text{ g cm}^{-3}.$$

Click on green square to return



Exercise 2(b)

Rearranging the equation for the **density**, we have

$$\text{mass} = \text{density} \times \text{volume} = 13.5 \times 25 = 337.5 \text{ g}.$$

Click on green square to return



Exercise 2(c)

The solution to this part of the exercise involves **two** calculations. First calculate the mass of 0.1 **moles** of acetone and then use this to find the **volume** of the substance. The **RMM** of acetone ($\text{C}_3\text{H}_6\text{O}$) is given by

$$\text{RMM} = 3 \times 12 + 6 \times 1 + 16 = 58.$$

The required **mass** is therefore

$$\text{mass} = \text{number of moles} \times \text{RMM} = 0.1 \times 58 = 5.8 \text{ g}.$$

As we have seen earlier,

$$\text{volume} = \frac{\text{mass}}{\text{density}} = \frac{5.8}{0.83} = 7 \text{ cm}^3.$$

Click on green square to return



Exercise 3(a) Since

$$\text{number of moles} = \frac{\text{volume} \times \text{molarity}}{1000}.$$

rearranging this gives

$$\begin{aligned} \text{volume} &= \frac{\text{number of moles} \times 1000}{\text{molarity}}. \\ &= \frac{7 \times 10^{-4} \times 10^3}{0.35} \\ &= \frac{7 \times 10^{-1}}{0.35} \\ &= \frac{0.7}{0.35} \\ &= 2 \text{ cm}^3. \end{aligned}$$

Click on green square to return



Exercise 3(b) Since

$$\text{number of moles} = \frac{\text{volume} \times \text{molarity}}{1000}.$$

we have, on rearranging the equation,

$$\begin{aligned} \text{molarity} &= \frac{\text{number of moles} \times 1000}{\text{volume}} \\ &= \frac{5 \times 10^{-2} \times 1000}{50} \\ &= \frac{5 \times 10^{-2} \times 10^3}{50} \\ &= \frac{5 \times 10}{50} = 1 \text{ M}. \end{aligned}$$

This is also 1 mol dm^{-3} .

Click on green square to return



Exercise 3(c) The pH is given by

$$\text{pH} = -\log_{10}[\text{H}^+].$$

Since the concentration is $[\text{H}^+]=1.0$, its pH is

$$\begin{aligned}\text{pH} &= \log_{10}[1.0] = 0, \\ \text{i.e. } \text{pH} &= 0.\end{aligned}$$

Click on green square to return



Exercise 4(a) From **Example 4** we have

$$\begin{aligned}\Delta H &= \Delta G + T\Delta S, \\ \Delta H - \Delta G &= T\Delta S, \\ \frac{\Delta H - \Delta G}{T} &= \Delta S.\end{aligned}$$

Click on green square to return



Exercise 5(a) From (2) we obtain

$$\Delta G^0 = -RT \ln K.$$

dividing both sides by $-RT$,

$$\frac{\Delta G^0}{-RT} = \ln K,$$

or
$$\ln K = -\frac{\Delta G^0}{RT}$$

Click on green square to return



Exercise 5(b) From the package on logarithms we have the formula for changing the bases of logarithms:

$$\log_a c = \log_a b \times \log_b c.$$

With $a = e$, $b = 10$, $c = x$, we have

$$\ln x = (\ln 10) \times (\log_{10} x)$$

so that, from (2), since $\ln 10 \simeq 2.3$,

$$\Delta G^0 = -2.3 RT \log_{10} K.$$

Click on green square to return



Solutions to Quizzes

Solution to Quiz:

The **RMM** for MgSO_4 is

$$24 + 32 + (4 \times 16) = 120.$$

Since

$$\text{number of moles} = \frac{\text{mass}}{\text{RMM}}$$

we have

$$\begin{aligned} \text{mass} &= \text{number of moles} \times \text{RMM} \\ &= 0.125 \times 120 \\ &= 15 \text{ g}. \end{aligned}$$

End Quiz

Solution to Quiz:

The solution to this problem involves two steps; first use the density to find the mass of 100 cm^3 of the substance, then use this to find the number of moles. The mass is

$$\text{mass} = \text{density} \times \text{volume} = 0.78 \times 100 = 78 \text{ g}.$$

The number of moles is then

$$\text{number of moles} = \frac{\text{mass}}{RMM} = \frac{78}{84} = 0.93$$

(Note: the RMM of cyclohexane is $(6 \times 12) + (12 \times 1) = 84$.)

End Quiz

Solution to Quiz:From **section 1**

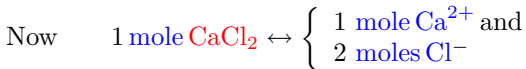
$$\text{no of moles} = \frac{\text{mass}}{\text{RMM}}$$

so 11.1 g of CaCl_2 (RMM=111 g mol⁻¹) corresponds to 11.1/111=0.1 moles of CaCl_2 .

The **number of moles** of a chemical substance contained in a solution is related to the molarity by

$$\text{number of moles} = \frac{\text{volume} \times \text{molarity}}{1000},$$

so that
$$\text{molarity} = \frac{\text{number of moles} \times 1000}{\text{volume}}.$$



Thus we obtain
$$\begin{aligned} \text{molarity of } \text{Ca}^{2+} &= (0.1 \times 100) / 2500 = 0.04. \\ \text{molarity of } \text{Cl}^- &= (0.2 \times 100) / 2500 = 0.08. \end{aligned}$$

End Quiz

Solution to Quiz:

From (1) and (2), we obtain

$$\begin{aligned}\Delta G^0 = -RT \ln K &= \Delta H^0 - T\Delta S^0, \\ \text{so that } RT \ln K &= -\Delta H^0 + T\Delta S^0, \\ \ln K &= \frac{-\Delta H^0 + T\Delta S^0}{RT} \\ &= \frac{-\Delta H^0}{RT} + \frac{\Delta S^0}{RT}.\end{aligned}$$

End Quiz

Solution to Quiz:

The **rate** equation is

$$\text{rate} = k[A]^x[B]^y,$$

and when $x = 0$ we have $[A]^0 = 1$. In this case the expression simplifies to

$$\text{rate} = k[B]^y.$$

End Quiz

Solution to Quiz:

Since

$$\text{Rate} = k[A]^x[B]^y,$$

we have, on taking logs,

$$\log \text{Rate} = \log k + x \log[A] + y \log[B].$$

(**Note:** Here we have used the following laws of logarithms

$$\log(A \times B) = \log A + \log B,$$

$$\log(A^k) = k \log A.$$

See the package on logarithms for details.)

End Quiz

Solution to Quiz:

In general, if $a = bx^y$, then $\ln a = \ln b + y \ln x$. From the Arrhenius equation

$$k = A \exp\left(-\frac{E_a}{RT}\right),$$

taking logarithms gives

$$\ln k = \ln A - \frac{E_a}{RT}.$$

(**Note:** Here we have used the following laws of logarithms

$$\log(A \times B) = \log A + \log B,$$

$$\log(A^k) = k \log A,$$

$$\ln(e) = \log_e(e) = 1.$$

See the package on logarithms for details.)

End Quiz

Solution to Quiz:

Using the result of the previous quiz we have

$$\begin{aligned}\ln k &= \ln A - \frac{E_a}{RT}, \\ \ln A - \ln k &= \frac{E_a}{RT}, \\ (\ln A - \ln k)RT &= E_a, \\ \text{or } E_a &= (\ln A - \ln k)RT, \\ &= \ln(A/k)RT, \\ &= RT \ln(A/k).\end{aligned}$$

(**Note:** Here we have used the following law of logarithms

$$\log \left(\frac{A}{B} \right) = \log A - \log B.$$

See the package on logarithms for details.)

End Quiz