Basic Mathematics

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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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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 $20\,\text{cm}^3$ has a mass of $20.4\,\text{g}$.

Solution Using the definition above,

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

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 $0.8\,\mathrm{g\,cm^{-3}}$.
(b) The mass of $25\,\mathrm{cm^3}$ of mercury if its density is $13.5\,\mathrm{g\,cm^{-3}}$
(c) The volume of 0.1 moles of acetone (C_3H_6O)if its density is $0.83\,\mathrm{g\ cm^{-3}}$.

Now try this short quiz.

Quiz If the density of cyclohexane (C_6H_{12}) is $0.78\,\mathrm{g\,cm^{-3}}$, which of the following is the number of moles in $100\,\mathrm{cm^3}$ 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 $1000\,\text{cm}^3$, or $1\,\text{dm}^3$, so the units are also in $\text{mol}\,\text{dm}^{-3}$.

Example 3 Calculate the number of moles of Cu^{2+} ions in $25\,\text{cm}^3$ 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

$$\Delta G = \Delta H - T\Delta S \tag{1}$$

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

$$\Delta G^0 = -RT \ln K \,, \tag{2}$$

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) $\ln K = \dfrac{\Delta H^0}{RT} - \dfrac{\Delta S^0}{R}\,,$

(b) $\ln K = \Delta H^0 - T\Delta S^0 + RT\,,$

(c) $\ln K = -\dfrac{\Delta H^0}{RT} + \dfrac{\Delta S^0}{R}\,,$

(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

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

where R is the universal gas constant.

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

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

Quiz Which of the following also represents the Arrhenius equation?

(a) $E_a = \ln(k/A)RT$,
(b) $E_a = \dfrac{\ln(A/k)}{RT}$,
(c) $E_a = \dfrac{\ln(A/k)}{RT}$,
(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

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

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Exercise 1(b)

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

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

we obtain

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

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Exercise 1(c)
The RMM for C_6H_6 is

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

Thus

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

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Exercise 2(a)

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

a rearrangement of the equation gives

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

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Exercise 2(b)

Rearranging the equation for the density, we have

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

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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 (C_3H_6O) is given by

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

The required mass is therefore

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

As we have seen earlier,

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

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Exercise 3(a) Since

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

rearranging this gives

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

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Exercise 3(b) Since

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

we have, on rearranging the equation,

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

This is also $1\,\mathrm{mol\,dm^{-3}}$.

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Exercise 3(c) The pH is given by

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

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

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

Click on green square to return ☐

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

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

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Exercise 5(a) From (2) we obtain

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

dividing both sides by -RT,

$$\begin{aligned} \frac{\Delta G^0}{-RT} &= \ln K\,, \\ \text{or} \qquad \ln K &= -\frac{\Delta G^0}{RT} \end{aligned}$$

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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

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Solutions to Quizzes

Solution to Quiz:

The RMM for $MgSO_4$ is

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

Since

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

we have

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

End Quiz

Solution to Quiz:

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

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

The number of moles is then

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

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

End Quiz

Solution to Quiz:
From **section 1**

$$\text{no of moles} = \frac{\text{m}ass}{\text{R}MM}$$

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

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

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

$$\text{Now} \qquad 1\,\text{mole}\,CaCl_2 \leftrightarrow \begin{cases} 1\ \text{mole}\,Ca^{2+} \text{ and} \\ 2\ \text{moles}\,Cl^{-} \end{cases}$$

Thus we obtain molarity of Ca^{2+}=(0.1×100)/2500 =0.04.
molarity of Cl^{-}=(0.2×100)/2500 =0.08.

End Quiz

Solution to Quiz:

From (1) and (2), we obtain

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

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

$$\begin{aligned} \log(A \times B) &= \log A + \log B\,, \\ \log\left(A^k\right) &= k\log A\,. \end{aligned}$$

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

$$\begin{aligned} \log(A \times B) &= \log A + \log B, \\ \log\left(A^k\right) &= k \log A, \\ \ln(e) = \log_e(e) &= 1. \end{aligned}$$

See the package on logarithms for details.)

End Quiz

Solution to Quiz:

Using the result of the previous quiz we have

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

(**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