Standard form and significant figures

Specification references

- *MS 0.1 Recognise and use expressions in standard and ordinary form*
- *MS 0.4 Use calculators to find and use power, exponential and logarithmic functions*
- *MS 1.1 Use an appropriate number of significant figures*

Learning objectives

After completing the worksheet you should be able to:

- convert between numbers in standard and ordinary form
- state numbers to a certain degree of accuracy.

Introduction

In the calculations you will be asked to perform as part of your AS studies you will need to be confident with both representing numbers in standard form and giving them to a certain number of significant figures.

When numbers are very large or very small they are written in **standard form**. In standard form a number is written in the format:

$$a \times 10^n \text{ where } 1 \leq a < 10 \text{ and } n \text{ is an integer.}$$

In an experiment, or from a calculation, you may only be able to give your answer with a certain amount of accuracy. This accuracy is shown by giving your answer to a certain number of **significant figures**.

Worked example: Standard form

Question

Express 0.00268 in standard form.

Answer

Step 1

Identify the value for '*a*.' In this case it will be 2.68.

Step 2

Work out how many places the decimal place must be moved to form this number.

$$0.00268$$

The decimal place must move 3 places to the right to become 2.68.

This number of places is the value for the integer '*n*.' If the decimal point moves to the right '*n*' is negative. If the decimal place moves to the left '*n*' is positive.

Step 3

Substitute your values into the general format, $a \times 10^n$

Therefore in standard form 0.00268 is 2.68×10^{-3}.

Worked example: Significant figures

Question

Express 0.56480900 to 3 significant figures.

Answer

Step 1

Identify the numbers which are significant using the rules below:

Rule 1 Any number that isn't 0 is significant.

Rule 2 Any 0 that is between two numbers that are not 0 is significant.

Rule 3 Any 0 that is before all the non-zero digits is not significant.

Rule 4 Any 0 that is after all of the non-zero digits is only significant if there is a decimal point.

In this case the significant numbers are 0.**564 809** 00.

Step 2

Identify the three most significant figures. These are the significant numbers which are furthest to the left (have the biggest values), i.e., 0.**564** 809 00.

Step 3

Look at the next number. If this number is 5 or above, then round up. If this number is 4 or less, do not round up.

In this case the next number is 8, so we round up to 0.**565**.

Questions

1 This question is about expressing numbers in standard form.
   a Express the following numbers in standard form.   (*4 marks*)
      i   0.0023
      ii 1032
      iii 275 000 0
      iv 0.000528
   b Write out the following numbers in ordinary form.   (*4 marks*)
      i 2.01×10^3
      ii 5.2×10^{-2}
      iii 8.41×10^2
      iv 1.00×10^{-4}

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   c For each of the pairs of numbers below identify which is the bigger number. (*3 marks*)

      i 1.43×10^{23} or 1.43×10^{24}

      ii 5.16×10^{-3} or 5.16×10^{-4}

      iii 12.4×10^{23} or 1.50×10^{24}

2 Express the following numbers to the number of significant figures indicated. (*6 marks*)

   a 4.74861 to two significant figures

   b 507980 to three significant figures

   c 809972 to three significant figures

   d 06.345 to three significant figures

   e 7840 to three significant figures

   f 0.007319 to three significant figures

3 Carry out the following calculations expressing the numbers in **standard form** to the degree of accuracy indicated: (*4 marks*)

   a $(4.567 \times 10^{5}) \times (2.13 \times 10^{-3})$ to three significant figures

   b $(1.567 \times 10^{3}) \div (2.245 \times 10^{-1})$ to four significant figures

   c $(5.4 \times 10^{-1}) \div (2.7 \times 10^{-3})$ to one significant figure

   d $(2.00 \times 10^{-2}) \times (2.00 \times 10^{-4})$ to three significant figures

Maths skills links to other areas

You will use these skills throughout the Amount of substance topics.

Answers

1 **a** **i** 2.3×10^{-3} *(1 mark)*

     ii 1.032×10^{3} *(1 mark)*

     iii 2.75×10^{6} *(1 mark)*

     iv 5.28×10^{-4} *(1 mark)*

  b **i** 2010 *(1 mark)*

     ii 0.052 *(1 mark)*

     iii 841 *(1 mark)*

     iv 0.0001 *(1 mark)*

  c **i** 1.43×10^{24} *(1 mark)*

     ii 5.16×10^{-3} *(1 mark)*

     iii 1.50×10^{24} *(1 mark)*

2

  a 4.7 *(1 mark)*

  b 508 000 *(1 mark)*

  c 810 000 *(1 mark)*

  d 6.35 *(1 mark)*

  e 7840 *(1 mark)*

  f 0.007 32 *(1 mark)*

3 **a** 9.73×10^{2} *(1 mark)*

  b 6.980×10^{3} *(1 mark)*

  c 2×10^{2} *(1 mark)*

  d 4.00×10^{-6} *(1 mark)*

Rates and order of reaction, rate-determining steps, and reaction mechanisms

Specification references

- *3.1.9*
- *MS0.0*
- *MS2.2, 2.3, 2.4*
- *MS3.3, 3.4*

Maths Skills for Chemistry references

- *6.4 Rates by inspection 1*
- *6.5 Rates by inspection 2*

Learning outcomes

After completing this worksheet, you should be able to:

- calculate the order of reaction for any reactant in a reaction
- write the rate equation for a reaction
- calculate the change in rate when the concentrations of the reactants in a rate equation are changed
- calculate the rate constant for a reaction and give its units
- link the rate equation with the mechanism of the reaction, and for some examples work out the mechanism.

Introduction

The equation that gives the relationship between the rate of reaction and the concentrations of the various reactants involved is called the rate equation.

For example:

$$\text{rate} = k\,[\mathbf{A}]^a\,[\mathbf{B}]^b\,[\mathbf{C}]^c$$

In this equation, *a* is the order of reaction with respect to reactant **A**, *b* is the order of reaction with respect to reactant **B**, and *c* is the order of reaction with respect to the reactant **C**. The overall order of the reaction $\square$ *a* + *b* + *c*. *k* is the rate constant. This is constant at any given temperature, but increases as temperature increases.

If *a* equals zero, then the order of reaction with respect to reactant **A** is zero order. If *a* $\square$ 1, then it is first order with respect to **A** etc. When you are calculating the order of reaction from a table of data, there are some basic principles you must remember.

Order of reaction	What does it mean?
Zero order	[**reactant**]^0 □ 1. This means that the rate of the reaction does not depend on the concentration of the reactant. For example, if the concentration of the reactant is doubled, then there is no effect on the rate.
First order	This means that the rate of the reaction is proportional to the concentration of the reactant. Therefore, if the concentration of the reactant is doubled, then the rate will double.
Second order	This means that the rate of the reaction is proportional to [**reactant**]^2. Therefore, if the concentration of the reactant is doubled, then the rate is increased fourfold. If the concentration of the reactant is trebled, then the rate of the reaction is increased ninefold.

If you have a rate equation where, for example, rate = k[**A**] [**B**]^2 [**C**] and **A** is doubled, **B** is also doubled, and **C** is trebled, then the effect on the rate is:

$$\frac{\text{rate 2}}{\text{rate 1}} = \frac{k[2\mathbf{A}][2\mathbf{B}]^2[3\mathbf{C}]}{k[\mathbf{A}][\mathbf{B}]^2[\mathbf{C}]} = 2 \times 4 \times 3 = 24$$

and therefore the rate is increased by a factor of 24.

The rate equation gives information about the mechanism of the reaction. For example, in the reaction involving the reactants **A**, **B**, and **C**, we can say that the rate-determining step in the equation, which is the slowest step, involves one molecule of **A**, two molecules of **B**, and one molecule of **C**.

Worked example

Question

The data in the table below shows the effect of the concentration of three reactants (**A**, **B**, and **C**) on the rate of a reaction. Use this data to:

a calculate the order of reaction with respect to each reactant

b write the overall rate equation

c calculate the value of the rate constant, k, and give its units

d calculate the effect on the rate if the concentration of all three reactants is increased fourfold.

Experiment	[A]/ mol dm^{-3}	[B]/ mol dm^{-3}	[C]/ mol dm^{-3}	Rate /mol dm^{-3} s^{-1}
1	1×10^{-3}	1×10^{-3}	1×10^{-3}	5×10^{-6}
2	2×10^{-3}	1×10^{-3}	1×10^{-3}	1×10^{-5}
3	2×10^{-3}	2×10^{-3}	1×10^{-3}	1×10^{-5}
4	1×10^{-3}	1×10^{-3}	3×10^{-3}	4.5×10^{-5}

Answer

a *Step 1*: Start with reactant **A** and choose two experiments where its concentration has changed, but the concentrations of the other reactants have not.

This means that we must use experiments 1 and 2. In these two experiments the concentration of **A** has doubled, and so has the rate as:

$$\frac{1 \times 10^{-5}}{5 \times 10^{-6}} = 2$$

Therefore, the reaction is first order with respect to **A**.

Step 2: Repeat with reactant **B**. The only two experiments where **B** changes are experiments 1 and 3, but so does the concentration of **A**. Comparing Experiment 1 to Experiment 3, the concentration of **A** doubles and so does the rate. But we already know that the reaction is first order with respect to **A** and this doubling of the rate must be due to the doubling of the concentration of **A**.

Therefore, changing the concentration of **B** has no effect on the rate, and the rate of the reaction is zero order with respect to **B**.

Step 3: For reactant **C**, we can use experiments 1 and 4. Here the concentration of **C** trebles, and the rate of the reaction increases nine times. Therefore, the order of reaction is second order with respect to **C**.

b Write the rate equation.

rate = k [**A**]^1 [**B**]^0 [**C**]^2 = k [**A**] [**C**]^2 (either expression is correct)

c To calculate the rate constant and its units, rearrange the rate equation:

$$k = \frac{\text{rate}}{[\textbf{A}][\textbf{C}]^2}$$

Now choose one of the experiments and use the data from that experiment. If we choose Experiment 1, then the following equation applies:

$$k = \frac{5 \times 10^{-6}}{10^{-3} \times (10^{-3})^2}$$

$$= \frac{5 \times 10^3 \text{ mol dm}^{-3}\text{s}^{-1}}{\text{mol dm}^{-3} \times (\text{mol dm}^{-3})^2}$$

$$= 5 \times 10^3 \text{ dm}^6 \text{ mol}^{-2} \text{ s}^{-1}$$

It does not matter in which order you write the units, but the convention is to put positive powers first.

d When calculating the effect on the rate of increasing all the concentrations fourfold:

- as the reaction is first order with respect to **A**, increasing the concentration of **A** by a factor of four also increases the rate by a factor of four

- as the reaction is second order with respect to **C**, increasing the concentration of **C** by a factor of four increases the rate by a factor of 4^2 or 16.

Taking both these factors into consideration, we can see that the rate is increased by a factor of 4×16 or 64.

Questions

1 Two substances, **P** and **Q**, react together: **P** + **Q** $\rightarrow$ products.

The data in the table below shows how the rate of the reaction depends on the concentrations of **P** and **Q**.

Experiment	[P]/ mol dm^{-3}	[Q]/ mol dm^{-3}	Rate/ mol dm^{-3} s^{-1}
1	2.00×10^{-3}	2.50×10^{-3}	6.6×10^{-6}
2	4.00×10^{-3}	2.50×10^{-3}	1.32×10^{-5}
3	2.00×10^{-3}	6.25×10^{-3}	1.65×10^{-5}

a Calculate the order of reaction with respect to both **P** and **Q**.

....

....

....

.... (*4 marks*)

b Write the rate equation for the reaction.

.... (*1 mark*)

c Calculate the value of the rate constant and give its units.

....

....

.... (*3 marks*)

d Calculate the effect on the rate if the concentrations of both **P** and **Q** are doubled.

....

.... (*2 marks*)

2 Three substances, **X**, **Y** and **Z**, undergo a chemical reaction. The data in the table below shows how the rate of the reaction depends on the concentrations of all three reactants.

Experiment	$[X]/$ mol dm^{-3}	$[Y]/$ mol dm^{-3}	$[Z]/$ mol dm^{-3}	Rate/ mol dm^{-3} s^{-1}
1	0.032	0.020	0.030	2.64×10^{-7}
2	0.064	0.020	0.030	1.06×10^{-6}
3	0.064	0.040	0.030	2.11×10^{-6}
4	0.032	0.020	0.060	5.28×10^{-7}

a Calculate the order of reaction with respect to **X**, **Y**, and **Z**.

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.... (*6 marks*)

b Write the rate equation for the reaction.

.... (*1 mark*)

c Calculate the value of the rate constant and give its units.

....

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.... (*3 marks*)

d Calculate the effect on the rate if the concentrations of **X** and **Y** are doubled, and the concentration of **Z** is trebled.

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.... (*4 marks*)

3 Hydrogen and nitrogen monoxide react together as follows:

$$2H_2(g) + 2NO(g) \rightarrow 2H_2O(g) + N_2(g)$$
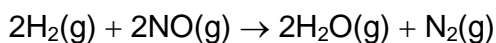
The rate equation for the reaction is:

rate $= k\,[\mathbf{H_2}]\,[\mathbf{NO}]^2$

a What happens to the rate of this reaction if the following changes take place:

i [**NO**] and [**H₂**] are both **doubled**

....

.... (*2 marks*)

ii [**NO**] is **halved** and [**H₂**] is **unchanged**?

....

.... (*2 marks*)

b The reaction mechanism consists of two steps. The first step is the rate-determining step. Use the data to write the mechanism.

....

....

.... (*3 marks*)

4 2-bromo-2-methylpropane, $(CH_3)_3CBr$, and iodide ions react as follows:

$$(CH_3)_3CBr + I^- \rightarrow (CH_3)_3CI + Br^-$$
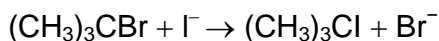
The data below shows how the rate of the reaction depends on the concentrations of $(CH_3)_3CBr$ and I^-.

Experiment	$[(CH_3)_3CBr]/$ mol dm^{-3}	$[I^-]/$ mol dm^{-3}	Rate/ mol dm^{-3} s^{-1}
1	0.016	0.020	1×10^{-6}
2	0.048	0.020	3×10^{-6}
3	0.048	0.060	3×10^{-6}
4	0.064	0.060	4×10^{-6}

a Calculate the order of the reaction with respect to the concentrations of 2-bromo-2-methylpropane and the iodide ions.

....

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....

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.... (*5 marks*)

b Calculate the rate constant for the reaction and give its units.

....

....

.... (*3 marks*)

c Give the mechanism for the reaction.

....

....

.... (*3 marks*)

Maths skills links to other areas

Calculating ratios comes into many areas of quantitative chemistry. For example, the redox chemistry of manganate(VII) requires the use of ratios in calculating the number of moles of each substance in the reaction. Calculating units is important with equilibrium constants.

Answers

1 a Using experiments 1 and 2, doubling **[P]** doubles the rate (*1 mark*). Therefore, the reaction is first order with respect to **B** (*1 mark*).

Using experiments 1 and 3, increasing **[Q]** by 2.5 times increases the rate by 2.5 times (*1 mark*). Therefore, reaction is first order with respect to **Q** (*1 mark*). (*4 marks*)

b Rate $= k$ **[P] [Q]** (*1 mark*)

c $k = \dfrac{\text{rate}}{\textbf{[P][Q]}} = \dfrac{6.6 \times 10^{-6}}{2 \times 10^{-3} \times 2.5 \times 10^{-3}} = 1.32$ (*2 marks*)

Units $= \dfrac{\text{mol dm}^{-3}\text{s}^{-1}}{\text{mol dm}^{-3} \times \text{ mol dm}^{-3}} = \text{dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ (*1 mark*) (*3 marks*)

d Doubling **[P]** doubles the rate and doubling **[Q]** also doubles the rate (*1 mark*). Therefore, rate increases by $2 \times 2 = 4$ times (*1 mark*). (*2 marks*)

2 a Using experiments 1 and 2, doubling **[X]** quadruples the rate (*1 mark*). Therefore, the reaction is second order with respect to **X** (*1 mark*).

Using experiments 1 and 3, both **[X]** and **[Y]** are doubled and the rate increases eightfold. Doubling **[X]** quadruples the rate and therefore, doubling **[Y]** leads to a doubling in the rate (*1 mark*), and so the reaction is first order with respect to **Y** (*1 mark*).

Using experiments 1 and 4, doubling **[Z]** also doubles the rate (*1 mark*) and therefore, reaction is first order with respect to **Z** (*1 mark*). (*6 marks*)

b Rate $= k$ **[X]**^{2} **[Y] [Z]** (*1 mark*)

c Rearranging the equation, and then using the data in Experiment 1:

$$k = \dfrac{\text{rate}}{\textbf{[X]}^2\textbf{[Y][Z]}} = \dfrac{2.64 \times 10^{-7}}{(0.032)^2(0.02)(0.03)}$$

$$= 0.430 \ (\textit{2 marks})$$

The units are $\dfrac{\text{mol dm}^{-3}\text{s}^{-1}}{(\text{mol dm}^{-3})^2(\text{mol dm}^{-3})(\text{mol dm}^{-3})} = \dfrac{\text{s}^{-1}}{(\text{mol dm}^{-3})^3} = \text{dm}^9 \text{ mol}^{-3} \text{ s}^{-1}$ (*1 mark*) (*3 marks*)

d Doubling **[X]** quadruples the rate (*1 mark*). Doubling **[Y]** doubles the rate (*1 mark*). Trebling **[Z]** trebles the rate (*1 mark*). Overall change in rate $= 4 \times 2 \times 3 = 24$ times (*1 mark*). (*4 marks*)

3 a i Doubling **[NO]** quadruples the rate. Doubling **[H₂]** doubles the rate (*1 mark*). Therefore, rate increases eightfold (*1 mark*).

(*2 marks*)

ii Halving [NO] changes the rate $\dfrac{1}{2} \times \dfrac{1}{2}$ times (*1 mark*) $= \dfrac{1}{4}$ times (*1 mark*) (*2 marks*)

b $2NO(g) + H_2(g) \rightarrow N_2O(g) + H_2O(l)$ (*1 mark*)   rate-determining step

$N_2O(g) + H_2(g) \rightarrow H_2O(l) + N_2(g)$ (*2 marks*)
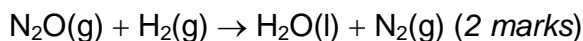
Note, the rate-determining step involves the two substances in the rate equation, and there are two molecules of N_2O because the rate is second order with respect to NO, and one molecule of H_2 because the rate is first order with respect to H_2.

If both sides of the equations are added we get:

$2NO(g) + H_2(g) + \cancel{N_2O(g)} + H_2(g) \rightarrow \cancel{N_2O(g)} + H_2O(l) + H_2O(l) + N_2(g)$

$2NO(g) + 2H_2(g) \rightarrow 2H_2O(l) + N_2(g)$
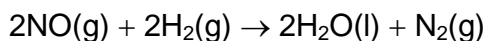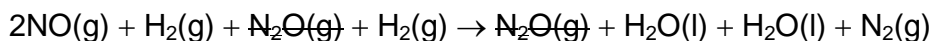
The N_2O is an intermediate in the reaction. (*3 marks*)

4 a Using experiments 1 and 2, if [$(CH_3)_3CBr$] trebles then the rate trebles (*1 mark*), therefore, the reaction is first order with respect to $(CH_3)_3CBr$ (*1 mark*).

Using experiments 2 and 3, if [I^-] is trebled there is no effect on rate (*1 mark*) and therefore, reaction is zero order with respect to I^- (*2 marks*). (*5 marks*)

b rate = k [$(CH_3)_3CBr$] $k = \dfrac{\text{rate}}{[(CH_3)_3CBr]}$ (*1 mark*)

Using experiment 1: $k = \dfrac{1 \times 10^{-6}}{0.016} = 6.25 \times 10^{-5} \dfrac{\text{mol dm}^{-3} \text{ s}^{-1}}{\text{mol dm}^{-3}}$ (*1 mark*)

$= 6.25 \times 10^{-5} \text{ s}^{-1}$ (*1 mark*) (*3 marks*)

c $(CH_3)_3CBr$ (*1 mark*) $\rightarrow (CH_3)_3C^+ + Br^-$ (*1 mark*) is the rate-determining step

Rate-determining step involves just $(CH_3)_3CBr$
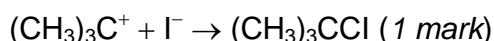
$(CH_3)_3C^+ + I^- \rightarrow (CH_3)_3CCl$ (*1 mark*) (*3 marks*)

Calculations involving dissociation constants and pH values of weak acids

Specification references

- *3.1.12*
- *MS0.0, 0.1, 0.4,*
- *MS2.1, 2.2, 2.3, 2.4, 2.5*

Maths Skills for Chemistry references

- *7.5 Calculating pH*
- *7.6 The acid dissociation constant*

Learning outcomes

After completing the worksheet, you should be able to:

- use the logarithmic expressions for pH and hydrogen ion concentration
- derive equations to work out the pH and hydrogen ion concentration of a weak acid
- use the expressions for pH, hydrogen ion concentration, and pK_a in calculations.

Introduction

The pH of an acid is related to its $[H^+(aq)]$ by the expression:

$$pH = -\log_{10} [H^+(aq)] \qquad \textbf{A}$$

For example, calculate the pH of a solution of 0.0001 mol dm^{-3} hydrochloric acid.

$pH = -\log_{10} [H^+ (aq)]$ and $[H^+ (aq)] = 0.0001$

When you use your calculator to find the pH value, you press the [log] button on your calculator, type in the number and then press [=]. Therefore $pH = -\log_{10}$ (0.0001) $= -(-4) = 4$

Another expression that you will use is:

$$[H^+ (aq)] = 10^{-pH} \qquad \textbf{B}$$

For example, what is the $[H^+(aq)]$ of an acid solution with a pH of 2.4. When you use your calculator to find $[H^+(aq)]$ using expression **B**, you press the [SHIFT] button followed by the [log] button, and then the number. In this example you will get $10^{-2.4}$ and the answer 3.98×10^{-3}. $[H^+(aq)] = 10^{-2.4}$

When you work out the pH of strong acids and bases, we can assume that they are fully dissociated in aqueous solution. For example, 0.1 mol dm^{-3} of hydrochloric acid has a hydrogen ion concentration of 0.1 mol dm^{-3}, because in aqueous solution all of the HCl molecules are dissociated into hydrogen and chloride ions.

Weak acids by definition are only partially dissociated in aqueous solution. Therefore, if you know the concentration of the weak acid, you do not automatically know the concentration of the hydrogen ions produced by its dissociation. To overcome this problem you have to use a model which in this case is a weak acid represented by the formula, HA. In aqueous solution, HA dissociates as follows:

$$HA\ (aq) \rightleftharpoons H^+(aq) + A^-(aq)$$
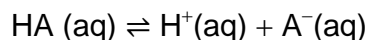
The equilibrium constant for this reaction is called the acid dissociation constant, K_a.

K_a is written as follows:

$$K_a = \frac{[H^+(aq)]_{eqm}[A^-(aq)]_{eqm}}{[HA(aq)]_{eqm}}\ \text{Units are mol dm}^{-3}$$

In this form we cannot use this expression because we do not know the values of $[H^+(aq)]_{eqm}$, $[A^-(aq)]_{eqm}$ and $[HA(aq)]_{eqm}$.

But we do know that $[H^+(aq)]_{eqm} = [A^-(aq)]_{eqm}$, because in the equilibrium there are equal numbers of both these ions. This means that the expression for K_a can be rewritten as:

$$K_a = \frac{[H^+(aq)]^2_{eqm}}{[HA(aq)]_{eqm}}\,\text{mol dm}^{-3} \qquad\qquad \textbf{A}$$

Also, since weak acids are only partially dissociated, then the $[HA(aq)]$ has hardly changed in value and $[HA(aq)]_{eqm} \sim [HA(aq)]_{start}$.

Therefore, $K_a = \dfrac{[H^+(aq)]^2_{eqm}}{[HA(aq)]_{start}}$

Rearranging this equation, we have $[H^+(aq)]^2_{eqm} = K_a \times [HA(aq)]_{start}$

And if we square root both sides

$$\mathbf{[H^+(aq)]_{eqm} = \sqrt{(K_a \times [HA(aq)]_{start})}} \qquad\qquad \textbf{B}$$

Another expression that you will need to know is pK_a.

$$\boldsymbol{pK_a = -\log_{10}K_a} \qquad\qquad \textbf{B}$$

This is a useful expression because it gives you some idea of the strength of an acid. The higher the value of pK_a, the weaker the acid:

$$\textbf{and } \boldsymbol{K_a = 10^{-pK_a}} \qquad\qquad \textbf{C}$$

Worked example

Question

The pK_a of a weak acid, HA, is 5.6.

a Calculate its K_a.

b Calculate the pH of a solution of HA with a concentration of 0.100 mol dm^{-3}.

Answer

Step 1

$K_a = 10^{-pK_a} = 2.51 \times 10^{-6}$

Step 2

$[H^+]^2 = K_a \times [HA]_{start}$ and $[H^+(aq)]_{eqm} = \sqrt{K_a \times [HA(aq)]_{start}}$

$= \sqrt{(2.51 \times 10^{-6} \times 0.100)} = 5.01 \times 10^{-4} \, mol \, dm^{-3}$

$pH = -\log_{10} 5.01 \times 10^{-4} = 3.3$

Questions

1 Calculate the pH for each of the following weak acid solutions.

	pK_a	Concentration mol dm^{-3}
a	4.8	0.02
b	6.7	9.94×10^{-5}
c	3.5	0.010
d	4.92	0.100

(*12 marks*)

2 Calculate the pK_a for each of the following weak acid solutions.

	pH	Concentration mol dm^{-3}
a	5.2	0.01
b	2.8	0.003
c	36.7	0.02
d	4.3	0.105

(*12 marks*)

Maths skills links to other areas

Logarithms are used in finding activation energy values from the Arrhenius equation.
They can also be used in resolving the order of reaction from concentration–rate data.

Answers

These answers include values that are part of the calculations on the way to the final answer. It may help the students identify where they may be going wrong.

Award 1 mark for each of the correct steps shown in the answer tables. Therefore for Question 1 there are 12 marks and the same for Question 2.

1.

Question	K_a/mol dm^{-3}	[H$^+$(aq)]/mol dm^{-3}	pH
a	1.58×10^{-5}	5.62×10^{-4}	3.25
b	2×10^{-7}	1.41×10^{-5}	4.84
c	3.16×10^{-4}	1.78×10^{-3}	2.75
d	1.20×10^{-5}	1.10×10^{-3}	2.96

2.

Question	[H$^+$(aq)]/mol dm^{-3}	K_a/mol dm^{-3}	pK_a
a	6.31×10^{-6}	3.98×10^{-9}	8.4
b	1.58×10^{-3}	8.37×10^{-4}	3.08
c	2×10^{-7}	2×10^{-12}	11.7
d	5.01×10^{-5}	2.39×10^{-8}	7.62

Ratios and amount of substance

Specification reference

- *3.1.2*
- *MS 0.2 Use ratios, fractions and percentages*
- *MS 1.1 Use an appropriate number of significant figures*
- *MS 2.2 Change the subject of an equation*

Maths Skills for Chemistry references

- *1.2 Amount of substance*

Learning objectives

After completing this worksheet you should be able to:

- use ratios from balanced chemical equations to calculate reacting masses
- state the answers to calculations to an appropriate number of significant figures.

Introduction

When an equation is balanced it gives us information about the amount of substances that react together and that are produced.

For example, look at the balanced equation for the reaction between magnesium and hydrochloric acid;

$$Mg(s) + 2\ HCl(aq) \rightarrow MgCl_2(aq) + H_2(g)$$
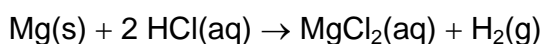
From the equation we know that 1 mol of Mg reacts with 2 mol of HCl to give 1 mol of $MgCl_2$ and 1 mol of H_2 gas. The magnesium reacts with the acid in a 1 : 2 molar ratio.

You'll notice that the total number of moles of reactant does not equal the total number of moles of product. This is because some species may contain more moles of certain atoms than others. For example, 1 mol of HCl contains 1 mol of Cl atoms whereas 1 mol of $MgCl_2$ contains 2 mol of Cl atoms. When balancing an equation we balance the number of individual atoms.

Worked example

Question

Calculate the mass of carbon monoxide needed to produce 11.2 g of iron from the reduction of iron oxide. The equation for the reaction is given below.

$$Fe_2O_3 + 3CO \rightarrow 2Fe + 3CO_2$$
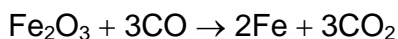
Answer

Step 1

Calculate the number of moles in 11.2 g of iron;

$$\text{Moles} = \frac{11.2 \text{ g}}{55.8 \text{ g mol}^{-1}} = 0.2007 \text{ mol}$$

Note: Carry intermediate numbers through as accurately as you can and where possible use the 'Ans' function on your calculator. In this example intermediate values have been written down to one significant figure more than you are going to give the final answer to, but have been carried through on the calculator using the 'Ans' function.

Step 2

Use ratios to determine the number of moles of carbon monoxide required to produce this number of moles of iron. The ratio of CO to Fe is:

3 mol CO : 2 mol of Fe

Divide both sides by 2 to find out how much CO is needed for 1 mol of Fe:

1.5 mol CO : 1 mol Fe

Multiply both sides by 0.2007 to find out how much CO is needed for 0.2007 mol of Fe:

0.3011 mol CO : 0.2007 mol Fe

Step 3

Convert the number of moles of CO into a mass of CO:

0.3011 mol × 28.0 g mol^{-1} = 8.430 g = 8.43 g (to 3 significant figures)

Give your final answer to the same degree of accuracy as the least accurate value given in the question. In this case 3 significant figures.

Questions

1   Sodium hydrogen carbonate can be neutralised by an excess of sulfuric acid as shown by the equation below:

$$2 \text{ NaHCO}_3 + \text{H}_2\text{SO}_4 \rightarrow \text{Na}_2\text{SO}_4 + 2 \text{ H}_2\text{O} + 2 \text{ CO}_2$$

   a   Calculate the number of moles in 105 g of NaHCO$_3$. (*1 mark*)

   b   Hence calculate the amount in moles of Na$_2$SO$_4$ which will be produced by the neutralisation of this sample of NaHCO$_3$. (*1 mark*)

   **c**   State the mass of Na$_2$SO$_4$ which will therefore be produced by this sample of NaHCO$_3$. (*1 mark*)

2   Lead nitrate will react with potassium iodide in a very unusual solid–solid reaction. The equation for the reaction is:

$$Pb(NO_3)_2 + 2\ KI \rightarrow PbI_2 + 2\ KNO_3$$
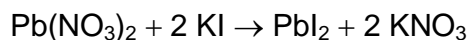
Calculate the mass of lead iodide that will be produced by the reaction of 14.1 g of potassium iodide with an excess of lead nitrate. (*3 marks*)

3 Solid copper can be prepared from copper oxide by its reaction with ammonia. The equation for the reaction is:
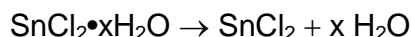
$$3\ CuO + 2\ NH_3 \rightarrow 3\ Cu + N_2 + 3\ H_2O$$
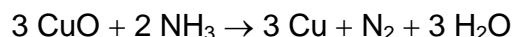
Calculate the mass of copper oxide which would react with 0.425 g of ammonia. (*3 marks*)

4 In a propane gas burner, the propane fuel undergoes complete combustion. Calculate the mass of oxygen required for the complete combustion of 62 g of propane. (*3 marks*)

5 Tin chloride exists as a hydrated salt. It can be dehydrated on heating:

$$SnCl_2 \bullet xH_2O \rightarrow SnCl_2 + x\ H_2O$$

If during the dehydration of a sample of hydrated tin chloride, 118.6 g of anhydrous tin chloride and 22.5 g of water are produced, calculate the value of x and hence state the formula of hydrated tin chloride. (*3 marks*)

6 Zinc chloride exists as a hydrated salt. It can be dehydrated on heating;

$$ZnCl_2 \bullet xH_2O \rightarrow ZnCl_2 + x\ H_2O$$
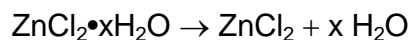
If 19.4 g of water are produced by the dehydration of 56.2 g of the hydrated salt, calculate the value of x and hence state the formula of hydrated zinc chloride. (*4 marks*)

Maths skills links to other areas

You will also need to be able to use ratios appropriately during amount of substance calculations involving gases and solutions and when determining empirical formula.

Answers

1 **a** moles of $NaHCO_3 = \dfrac{105\,g}{84.0\,g\,mol^{-1}} = 1.25$ mol (*1 mark*)

b 2 $NaHCO_3$: 1 Na_2SO_4, $\therefore$ 1 $NaHCO_3$: 0.5 Na_2SO_4 and
$\therefore$ 1.25 mol $NaHCO_3$: 0.625 mol Na_2SO_4 (*1 mark*)

c 0.625 mol $\times$ 142.1 g mol^{-1} = 88.81 g = 88.8 g (to 3 significant figures) (*1 mark*)

2 No. of moles in 14.1 g of KI = $\dfrac{14.1\,g}{166.0\,g\,mol^{-1}} = 0.08494$ mol (*1 mark*)

2KI : 1PbI$_2$, therefore moles of PbI$_2$ produced = $\dfrac{0.08494\,mol}{2} = 0.04247$ mol (*1 mark*)

Mass of PbI$_2$ produced = 0.04247 mol $\times$ 461.0 g mol^{-1} = 19.57 g = 19.6 g
(to 3 significant figures) (*1 mark*)

3 No. of moles in 0.425 g of NH_3 = $\dfrac{0.425\,g}{17.0\,g\,mol^{-1}} = 0.025$ mol (*1 mark*)

3 CuO : 2 NH_3, therefore moles of CuO needed = $\dfrac{0.025}{2} \times 3 = 0.0375$ mol (*1 mark*)

Mass of CuO needed = 0.0375 mol $\times$ 79.5 g mol^{-1} = 2.981 g = 2.98 g (to 3
significant figures). (*1 mark*)

4 $C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$ (*1 mark*)

No. of moles in 62 g of propane = $\dfrac{62\,g}{44.0\,g\,mol^{-1}} = 1.409$ mol (*1 mark*)

1 C_3H_8 : 5 O_2, therefore moles of O_2 needed = 1.409 mol $\times$ 5 = 7.045 mol (*1 mark*)

Mass of O_2 needed = 7.045 mol $\times$ 32.0 g mol^{-1} = 225 g = 230 g (to 2 significant
figures). (*1 mark*)

5 No. of moles in 118.6 g of $SnCl_2$ = $\dfrac{118.6\,g}{189.7\,g\,mol^{-1}} = 0.6252$ mol (*1 mark*)

No. of moles in 22.5 g of H_2O = $\dfrac{22.5\,g}{18.0\,g\,mol^{-1}} = 1.25$ mol (*1 mark*)

If 1 $SnCl_2$: x H_2O = 0.625 mol $SnCl_2$: 1.25 mol H_2O = 1 mol $SnCl_2$: 2 mol H_2O
then x = 2
The formula for hydrated tin chloride is $SnCl_2 \cdot 2H_2O$. (*1 mark*)

6 Mass of anhydrous $ZnCl_2$ produced = 56.2 g – 19.4 g = 36.8 g (by the
conservation of
mass rule).

No. of moles in 36.8 g of $ZnCl_2 = \dfrac{36.8 \text{ g}}{136.4 \text{ g mol}^{-1}} = 0.2697$ mol   (*1 mark*)

No. of moles in 19.4 g of $H_2O = \dfrac{19.4 \text{ g}}{18.0 \text{ g mol}^{-1}} = 1.077$ mol   (*1 mark*)

If 1 $ZnCl_2$: x H_2O = 0.2697 mol $ZnCl_2$: 1.077 mol H_2O = 1 $ZnCl_2$: 3.99 H_2O then
x = 4

The formula for hydrated zinc chloride is $ZnCl_2 \bullet 4H_2O$.   (*1 mark*)

Shapes of molecules

Specification reference

- *3.1.3.5*
- *MS 4.1 Use angles and shapes in regular 2D and 3D structures*
- *MS 4.2 Visualise and represent 2D and 3D forms including 2D representations of 3D objects*

Maths Skills for Chemistry references

- *2.1 Shape of simple molecules*

Learning objectives

After completing the worksheet you should be able to:

- *predict the shapes of, and bond angles in, simple molecules and ions*
- *visualise 3D shapes of simple molecules and ions and represent them in a 2D form.*

Introduction

We can measure angles in degrees, °, where 360° is equal to one complete circle. We use degrees in chemistry when describing the shape of a molecule.

The shape of a molecule or molecular ion can be predicted if the connectivity of the atoms and the arrangement of electron pairs around the central atom is known. The electron pairs repel each other and as a result take up a geometry where they are as far apart as possible and therefore have the lowest energy. This is called electron pair repulsion theory. Note that atoms in Groups 5, 6, 7 and 0 and Period 3 onwards can hold more than 8 electrons in their outer shell. They can 'expand the octet'.

Table 1 shows the optimised geometries for arranging between 2 and 6 electron pairs around a central atom. A dashed bond represents a bond going into the page, a wedge bond represents a bond coming out of the page. The **bond angle** is the angle between any three atoms / any two bonds.

When a molecule contains lone pairs, lone pairs are more repulsive than bonding pairs as a result of being closer to the nucleus of the atom. This distorts the basic shape described in Table 1 and reduces the bond angle between bonding pairs by 2.5°.

Table 1 *Optimised geometries of molecules containing two to six bonding pairs
around a central atom*

No. of electron pairs	2	3	4	5	6
Shape	X—A—X				
Name	linear	trigonal planar	tetrahedral	triangular bipyramid	octahedral
Bond angle(s)	180°	120°	109.5° or 109°	90° and 120°	90°

Worked example

Question

Draw a '*dot-and-cross*' diagram for PCl_3 and hence determine the molecule's overall shape and bond angle.
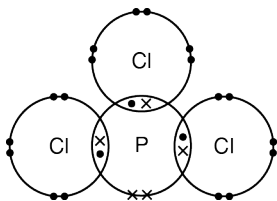
Answer

Step 1

Determine the number of outer shell (valence) electrons in each of the atoms in the molecule:

Phosphorus has 5 valence electrons; chlorine has 7 valence electrons.

Step 2

Draw a dot-and-cross diagram to show the bonding in the molecule.

Step 3

Count the number of electron pairs around the central atom. Use the table and this number of electron pairs to determine the basic geometry of the molecule.

In this case there are four pairs of electrons around the central phosphorus and so the electron pairs take up a tetrahedral structure;
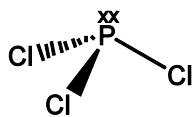
Therefore the shape of the molecule is either '*tetrahedral*' or if we are looking only at the atoms, the shape is '*triangular pyramidal*'.

Step 4

Calculate the bond angle.

The standard bond angle for a tetrahedral structure is 109.5°. However, lone pairs repel more than bonding pairs, and reduce the bond angle by 2.5°. Hence for PCl_3, the bond angle is 109.5° − 2.5° = 107°.

Questions

1 Draw 'dot-and-cross diagrams' for each of the molecules below.

Use the dot-and-cross diagrams to determine the overall shape (with respect to the number of pairs of electrons) and bond angle(s) for each of the molecules.

Show the bond angles on a 2D representation of the 3D structure. (*4 marks each*)

  a $AlCl_3$

  b NH_3

  c PF_5

  d $BeCl_2$

  e ClF_3

2 Draw 'dot-and-cross diagrams' for each of the molecular ions below.

Use these to determine the overall shape (with respect to the number of pairs of electrons) and bond angle(s) for each of the molecular ions.

Show the bond angles on a 2D representation of the 3D structure.

HINT For a negative molecular ion, add one extra electron for each negative charge. For a positive molecular ion, remove one electron for each positive charge. (*4 marks each*)

  a PH_4^+

  b H_3O^+

  c IF_6^+

  d AsF_6^-

  e $XeCl_3^-$

3 *From AQA Chemistry Unit 1 Foundation Chemistry CHEM1 January 2013 (Question 6)*

Chlorine can form molecules and ions that contain only chlorine, or that contain chlorine combined with another element.

Use your understanding of the electron pair repulsion theory to draw the shape of the $AsCl_3$ molecule and the shape of the Cl_3^+ ion.

Include any lone pairs of electrons that influence the shape.

Name the shape made by the atoms in the $AsCl_3$ molecule and in the Cl_3^+ ion.

(*4 marks*)

Maths skills links to other areas

You will also be required to visualise and draw the shapes of molecules when studying isomers in the organic section of the course.

Answers

4 For each part of the question award a maximum of four marks from:

- correct dot-and-cross diagram   (*1 mark*)
- correct diagram of 3D structure   (*1 mark*)
- correct shape of the molecule stated   (*1 mark*)
- correct bond angle   (*1 mark*)
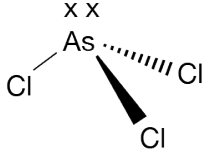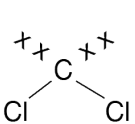
	Dot-and-cross diagram	3D diagram	Shape of the molecule	Bond angle /°
a			trigonal planar	120
b			tetrahedral OR triangular pyramidal	107
c			triangular bipyramid	90 and 120
d			linear	180
e			triangular bipyramid	120

5 For each part of the question award a maximum of three marks from:
- correct diagram of 3D structure   (*1 mark*)
- correct shape of the molecule stated   (*1 mark*)
- correct bond angle   (*1 mark*)

	Dot and cross diagram	3D diagram	Shape of the molecule	Bond angle/°
a			tetrahedral	109.5
b			tetrahedral	107
c			octahedral	90
d			octahedral	90
e			octahedral	90

6 *From AQA Chemistry Unit 1 Foundation Chemistry CHEM1 January 2013*
(Question 6)

Answer	Marks	Guidance
x x As ......⁗ Cl Cl Cl Cl Triangular pyramid(al) ⁺ ˣˣ C ˣˣ Cl Cl Bent / V-shaped	1 1 1 1	Mark is for 3 As-Cl bonds and 1 lone pair Mark is for 2 Cl-Cl bonds and 2 lone pairs Do not penalise if + not shown Not trigonal

The Maxwell–Boltzmann distribution

Specification references

- *3.1.5.3*
- *3.1.5.5*
- *MS3.1*

Maths Skills for Chemistry references

- *6.1 Boltzmann distributions*

Learning objectives

After completing the worksheet you should be able to:

- interpret information provided in a graphical format
- explain, using Maxwell–Boltzmann distributions, the effect of temperature and a catalyst on the rate of a reaction.

Introduction

A distribution curve is a map of occurrences between two variables. It is similar to a frequency histogram.

From a distribution curve it is possible to determine the most probable value (the **mode**) for a set of data. The shape of the curve provides information about the distribution of the variables within the sample. The area under the curve is an indication of the size of sample.

Worked example: Distribution curves

Question

The graph below shows the distribution of particle sizes within a sample of powder.
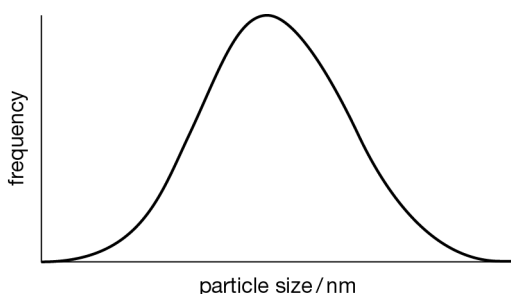
particle size / nm

On the graph:

a label the most probable particle size

---

b sketch a curve to show how the distribution would change if there were more large particles in the sample, but the overall number of particles in the sample didn't change.

Answer

a The most probable particle size is the particle size with the highest frequency.

most probable particle size
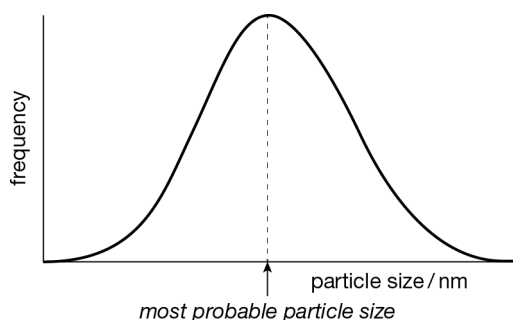
b If there were more large particles in the sample, the curve would be skewed towards the right (higher particle size). Note:

- The curve will still pass through (0,0) as no particles have no size.
- The area under the curve would not change as the sample size is the same.
- The most probable particle size will be larger.
- The frequency of the most probable particle size will be lower. (This must be the case if the area remains constant.)
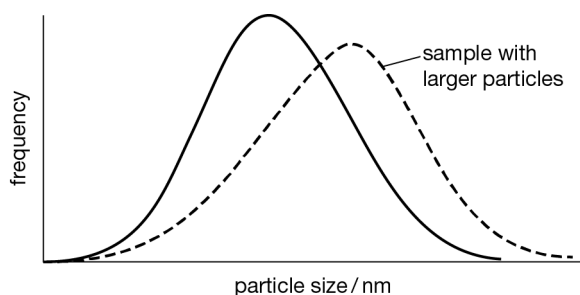
Questions

1 The diagram below shows the Maxwell-Maxwell–Boltzmann distribution of molecular energies in a sample of gas.

This resource sheet may have been changed from the original
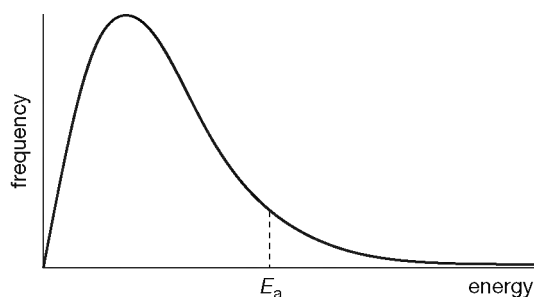
a Indicate on the graph:

    i the most probable energy of the particles   (*1 mark*)

    ii an approximate position for the average energy of the particles.   (*1 mark*)

b E_a represents the activation energy that the particles need in order to react. Indicate on the graph, by shading, the number of particles with enough energy to react.   (*1 mark*)

c A catalyst is added to the reaction. Indicate with E_{cat} a possible energy for the new activation energy for the reaction with the catalyst, and explain the effect of the catalyst on the rate of reaction.   (*3 marks*)

2 The curve below shows the distribution of molecular energies in a gas at temperature, T_1.
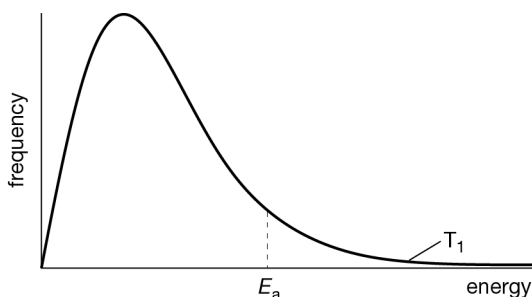
a Draw on the graph a second curve to represent the same sample of gas at a higher temperature. Label this curve T_2.   (*2 marks*)

b Explain any changes to:

    i the most probable energy of the particles   (*2 marks*)

    ii the total area under the curve   (*2 marks*)

    iii the number of particles with the activation energy, E_a (*2 marks*)

    iv the starting point of the curve   (*2 marks*)

    v the end point of the curve.   (*2 marks*)

Maths skills links to other areas

You will also be required to interpret graphical data when interpreting spectra and when studying patterns in ionisation energies.

Answers

1

most probable   average
energy   energy

E_{cat} E_a energy
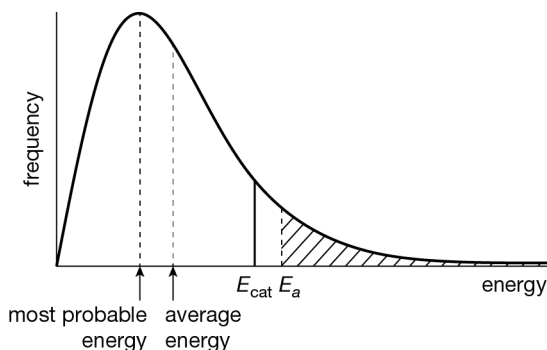
a **i**   The most probable energy is the energy with the highest frequency. (*1 mark*)

   ii The average energy will lie to the right of the most probable energy for this distribution because there are more particles (a bigger area under the curve) to the right of the most probable energy. (*1 mark*)

b The number of particles with the activation energy or above is indicated by shading under the curve to the right of the activation energy. (*1 mark*)

c A catalyst lowers the activation energy for a reaction. The number of particles with the activation energy is now vastly increased (the area to the right of the activation energy is now significantly larger) and hence there is a higher frequency of successful collisions. (*3 marks*)

2 a

E_a energy (*2 marks*)
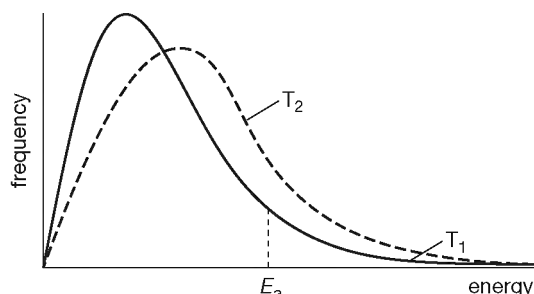
b **i**   The most probable energy of the particles will increase as the sample is at higher temperature. (*2 marks*)

   ii The total area will not change as it is the same sample of gas and so the overall number of particles has not changed. (*2 marks*)

   iii The number of particles with the activation energy will increase as the distribution
is skewed to the right. The area under the curve to the right of the activation energy is bigger at T_2 than at T_1. (*2 marks*)

   iv Both curves start at (0,0) as no particles have no energy. (*2 marks*)

   v Both curves never touch the *x*-axis as a very few particles will have very high energies indeed (there is no upper limit). (*2 marks*)

Titration calculations

Specification reference

- *3.1.7*
- *MS 0.0 Recognise and make use of appropriate units in calculations*
- *MS 0.1 Recognise and use expressions in decimal and ordinary form*
- *MS 1.1 Use an appropriate number of significant figures*
- *MS 1.2 Find arithmetic means*
- *MS 2.2 Change the subject of an equation*

Maths Skills for Chemistry references

- *1.9 Titrations*

Learning objectives

After completing the calculation sheet you should be able to:

- select appropriate titration data and use this data to calculate a mean titre
- determine the concentration of an unknown solution of acid or alkali from titration data, reporting results to an appropriate number of significant figures.

This worksheet builds on your understanding of significant figures, balancing equations, units and concentration, and ratios and amount of substance.

Introduction

A titration is used to measure the volume of one solution that reacts with another solution. It allows you to determine the precise endpoint of a reaction and hence is a useful analytical tool.

When analysing a substance by titration, the titration is repeated until two *concordant* titres are achieved. These must be within 0.10 cm^3 of each other. The mean of the concordant titres is then used in any calculations. The mean titre is calculated by finding the sum of all concordant titres and dividing by the number of concordant titres in the sum:

$$\text{Mean titre} = \frac{\text{Sum of all concordant titres}}{\text{Number of concordant titres}}$$

Worked example

Question

A solution of sulfuric acid of unknown concentration was titrated against 25.0 cm^3 of a 0.105 mol dm^{-3} solution of sodium hydroxide. The results of the analysis are shown in the table.

This resource sheet may have been changed from the original

	Trial	1	2	3
Final burette reading / cm^3	22.55	41.60	20.30	39.40
Initial burette reading / cm^3	2.05	22.55	1.40	20.30
Titre / cm^3	20.50	19.05	18.90	19.10

Calculate the concentration of the sulfuric acid solution.

Answer

Step 1

Identify the concordant titres. These are the titres within 0.1 cm^3 of each other.

In this case these are 19.05 cm^3 and 19.10 cm^3.

Step 2

Calculate the mean titre from the two or more concordant titres:

$$(19.05 \text{ cm}^3 + 19.10 \text{ cm}^3) \div 2 = 19.075 \text{ cm}^3$$

HINT: This value should lie between your concordant titres.

Step 3

Write a balanced symbol equation for the reaction occurring.

$$2NaOH + H_2SO_4 \rightarrow Na_2SO_4 + 2H_2O$$
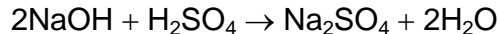
Step 4

Calculate the no. of moles in the solution with a known concentration.

In this case, the no. of moles in 25.0 cm^3 of 0.105 mol dm^{-3} NaOH:

$$\text{moles} = \text{concentration (mol dm}^{-3}) \times \text{volume (dm}^3)$$

NOTE: The volume must be expressed in dm^3, where 1 dm^3 = 1000 cm^3.
Therefore 25.0 cm^3 = 0.025 dm^3.

$$\text{moles of NaOH} = 0.105 \text{ mol dm}^{-3} \times 0.025 \text{ dm}^3 = 2.625 \times 10^{-3} \text{ mol}$$

Step 5

Use the stoichiometry of the reaction to determine the number of moles of sulfuric acid which reacts with 2.625×10^{-3} mol of NaOH exactly.

$$2NaOH : 1H_2SO_4$$
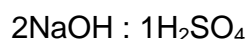
Therefore, the no. of moles of H_2SO_4 required to exactly neutralise 2.625×10^{-3} mol

of NaOH $= \dfrac{2.625 \times 10^{-3} \text{ mol}}{2}$

$$= 1.3125 \times 10^{-3} \text{ mol}.$$

Step 6

Calculate the concentration of the sulfuric acid.

The mean titre of sulfuric acid contains 1.3125×10^{-3} mol.

Therefore $19.075\,cm^3 = 0.019075\,dm^3$ of the sulfuric acid contains 1.3125×10^{-3} mol of acid.

Substitute these values into the equation for concentration:

$$\text{Concentration}\ (mol\,dm^{-3}) = \frac{\text{number of moles (mol)}}{\text{volume (dm}^3)}$$

$$\text{Concentration}\ (mol\,dm^{-3}) = \frac{1.3125 \times 10^{-3}\ \text{mol}}{0.019075\ \text{dm}^3}$$

$$= 0.06881\ mol\,dm^{-3}$$

Step 7

Give your final answer to the same degree of accuracy (significant figures) as the information given in the question, in this case three significant figures.

The concentration of the sulfuric acid is $0.0688\,mol\,dm^{-3}$.

Questions

1 A solution of hydrochloric acid of unknown concentration was titrated against $25.0\,cm^3$ of a $0.210\,mol\,dm^{-3}$ solution of sodium hydroxide. The results of the analysis are shown in the table.

	Trial	1	2	3
Final burette reading / cm³	17.45	28.65	15.70	30.90
Initial burette reading / cm³	1.00	32.90	0.40	15.70
Titre / cm³	16.45	15.45	15.30	15.20

  a Write a balanced symbol equation for the neutralisation reaction. (*1 mark*)
  b Calculate the mean titre of hydrochloric acid. (*1 mark*)
  c Calculate the number of moles in $25.0\,cm^3$ of a $0.210\,mol\,dm^{-3}$ solution of NaOH. (*1 mark*)
  d Use your answer to parts **a** and **c** to determine the no. of moles of hydrochloric acid in the average titre. (*1 mark*)
  e Use your answers to parts **b** and **d** to calculate the concentration of the hydrochloric acid. (*1 mark*)

2 A solution of sulfuric acid of unknown concentration was titrated against 25.0 cm^3 of a 0.100 mol dm^{-3} solution of calcium hydroxide. The equation for the neutralisation is:

$$H_2SO_4 + Ca(OH)_2 \rightarrow CaSO_4 + 2\,H_2O$$
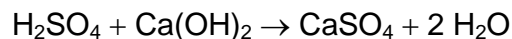
The results of the analysis are shown in the table.

	Trial	1	2	3
Final burette reading / cm^3	32.05	17.45	28.45	28.30
Initial burette reading / cm^3	0.05	0.10	0.10	0.00
Titre / cm^3	32.00	28.55	28.35	28.30

Calculate the concentration of the sulfuric acid solution. (*4 marks*)

3 $2\,NaHCO_3 + H_2SO_4 \rightarrow Na_2SO_4 + 2\,H_2O + 2\,CO_2$

25.0 cm^3 of a 0.200 mol dm^{-3} solution of sodium hydrogen carbonate was titrated against a solution of sulfuric acid of unknown concentration. The results of the titration are shown in the table below.

	Trial	1	2	3
Final burette reading / cm^3	17.20	32.25	15.25	31.40
Initial burette reading / cm^3	0.10	17.20	0.10	16.30
Titre / cm^3	17.10	15.05	15.15	15.10

Calculate the concentration of the sulfuric acid. (*4 marks*)

4 20.0 cm^3 of ammonia solution NH_4OH, was placed in a conical flask and titrated against a 0.250 mol dm^{-3} solution of hydrochloric acid. The results are shown below.

	Trial	1	2	3	4
Final burette reading / cm^3	35.10	32.25	32.35	32.15	32.05
Initial burette reading / cm^3	0.10	0.20	0.10	0.25	0.00
Titre / cm^3	35.00	32.05	32.25	31.90	32.05

   a Construct an equation for the neutralisation reaction (*1 mark*)

   b Calculate the concentration of the ammonia solution. (*4 marks*)

Maths skills links to other areas

These calculations use many of the mathematical skills you have encountered so far including using numbers in standard form, giving answers to an appropriate degree of accuracy and using ratios to determine numbers of moles reacting. These skills will be required throughout your A Level Chemistry studies.

You will be required to use weighted means when calculating atomic mass from isotopic abundances.

Answers

1 **a** $HCl + NaOH \rightarrow NaCl + H_2O$ (*1 mark*)

  b Concordant titres are $15.30 \, cm^3$ and $15.20 \, cm^3$

  Mean titre $= \dfrac{15.30 \, cm^3 \times 15.20 \, cm^3}{2}$

  $= 15.25 \, cm^3$ (*1 mark*)

  c moles of NaOH $= 0.025 \, dm^3 \times 0.210 \, mol \, dm^{-3}$

  $= 5.25 \times 10^{-3} \, mol$ (*1 mark*)

  d 1 mol HCl : 1 mol NaOH therefore moles of HCl $= 5.25 \times 10^{-3} \, mol$ (*1 mark*)

  e Concentration $= \dfrac{5.25 \times 10^{-3} \, mol}{0.01525 \, dm^3}$

  $= 0.3442 \, mol \, dm^{-3}$

  $= 0.344 \, mol \, dm^{-3}$ (to 3 significant figures). (*1 mark*)

2 Concordant titres are $28.35 \, cm^3$ and $28.30 \, cm^3$

Mean titre of sulfuric acid $= 28.325 \, cm^3$ (*1 mark*)

Moles of $Ca(OH)_2 = 0.025 \, dm^3 \times 0.100 \, mol \, dm^{-3}$

  $= 2.5 \times 10^{-3} \, mol$ (*1 mark*)

1 mol H_2SO_4 : 1 mol $Ca(OH)_2$ therefore moles of $H_2SO_4 = 2.5 \times 10^{-3} \, mol$ (*1 mark*)

Concentration of $H_2SO_4 = \dfrac{2.5 \times 10^{-3} \, mol}{0.028325 \, dm^3}$

  $= 0.08826 \, mol \, dm^{-3}$

  $= 0.0882 \, mol \, dm^{-3}$ (to 3 significant figures). (*1 mark*)

3 Concordant titres are $15.05 \, cm^3$, $15.15 \, cm^3$ and $15.10 \, cm^3$

Mean titre of sulfuric acid $= 15.10 \, cm^3$ (*1 mark*)

Moles of $NaHCO_3 = 0.025 \, dm^3 \times 0.200 \, mol \, dm^{-3}$

  $= 5.00 \times 10^{-3} \, mol$ (*1 mark*)

2 mol $NaHCO_3$: 1 mol H_2SO_4 therefore moles of $H_2SO_4 = 2.5 \times 10^{-3} \, mol$ (*1 mark*)

Concentration of $H_2SO_4 = \dfrac{2.5 \times 10^{-3} \, mol}{0.0151 \, dm^3}$

  $= 0.1655 \, mol \, dm^{-3}$

  $= 0.166 \, mol \, dm^{-3}$ (to 3 significant figures). (*1 mark*)

4 **a** $NH_4OH + HCl \rightarrow NH_4Cl + H_2O$ (*1 mark*)

  b Concordant titres are $32.05 \, cm^3$ and $32.05 \, cm^3$

  Mean titre of HCl $= 32.05 \, cm^3$ (*1 mark*)

  Moles of HCl $= 0.03205 \, dm^3 \times 0.250 \, mol \, dm^{-3}$

  $= 8.0125 \times 10^{-3} \, mol$ (*1 mark*)

  1 mol NH_4OH : 1 mol HCl therefore moles of HCl $= 8.0125 \times 10^{-3} \, mol$ (*1 mark*)

Concentration of ammonia solution $= \dfrac{8.0125 \times 10^{-3} \text{ mol}}{0.0200 \text{ dm}^3}$

$= 0.04006 \text{ mol dm}^{-3}$

$= 0.0400 \text{ mol dm}^{-3}$ (to 3 significant figures).   (*1 mark*)

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Calculations involving buffer solutions

Specification references

- *3.1.12*
- *MS0.1, 0.4*
- *MS2.4, 2.5*

Maths Skills for Chemistry references

- *7.9 pH of buffers*

Learning outcomes

After completing this worksheet, you should be able to:

- adapt the equation for the acid dissociation constant in order to find the pH of a buffer solution
- calculate the pH of a buffer solution from the concentrations of the weak acid and its conjugate base
- calculate the concentrations of either the acid or salt contained in a buffer solution given all the other variables.

Introduction

Buffer solutions are studied after pH and weak acids and acid dissociation constants. Therefore, you should be familiar with the expressions for pH, [H^+(aq)] (in terms of pH), K_a, and pK_a.

A buffer solution is a mixture of a weak acid and its conjugate base. The conjugate base is in the form of a salt of the acid. An example of a buffer solution is a solution of ethanoic acid and sodium ethanoate. The ethanoate ion is the conjugate base.

The equation for the acid dissociation constant of a weak acid, HA, is as follows:

$$K_a = [H^+(aq)] \frac{[A^-(aq)]}{[HA(aq)]}$$

Because we are usually interested in the pH of the solution, we need to know [H^+(aq)].

Rearranging this equation so that the [H^+(aq)] is the subject of the equation we multiply both sides by [HA] and divide both sides by [A^-].

The rearranged equation is: $[H^+(aq)] = K_a \times \dfrac{[HA(aq)]}{[A^-(aq)]}$

And since [HA(aq)] = concentration of the acid and [A^-(aq)] = concentration of the salt we have:

$$[H^+(aq)] = K_a \times \frac{[acid]}{[salt]}$$

And this equation can be used to find the pH of a buffer from the $[H^+(aq)]$.

An interesting development of this equation is that when $[HA(aq)] = [A^-(aq)]$. In this case $[H^+(aq)] = K_a$, and when taking minus logs on both sides:

$$pH = -\log_{10}K_a = pK_a$$

This means that if we add together equal volumes of equimolar solution of a weak acid and its salt, and measure the pH of the resulting solution, that will give us the pK_a of the acid.

Worked example

Question

1 A weak acid has a K_a equal to 6.2×10^{-6}. What is the pH of a buffer solution where the concentration of the acid is 0.100 mol dm^{-3} and the salt has a concentration of 0.0660 mol dm^{-3}?

Answer

Use the equation above in **bold**.

$$[H^+(aq)] = K_a \times \frac{[acid]}{[salt]} = 6.2 \times 10^{-6} \times \frac{0.1}{0.0660} = 9.40 \times 10^{-6}$$

$$pH = -\log_{10}[H^+(aq)] = -\log_{10} 9.40 \times 10^{-6} = 5.03$$

Question

2 A buffer solution has a pH of 7.9. The concentration of the acid is 0.0500 mol dm^{-3} and its pK_a is equal to 8.3. What is the concentration of the salt solution in this buffer mixture?

Answer

Step 1 Use the equation above in **bold**.

$$[H^+(aq)] = K_a \times \frac{[acid]}{[salt]}$$

Step 2 Rearrange the equation to make [salt] the subject of the equation.

$$[salt] = K_a \times \frac{[acid]}{[H^+(aq)]}$$

Step 3 Calculate the values of K_a and $[H^+(aq)]$ and then substitute them into the equation.

$K_a = 10^{-pK_a} = 10^{-8.3} = 5.01 \times 10^{-9}$ mol dm^{-3}

and $[H^+(aq)] = 10^{-pH} = 10^{-7.9} = 1.26 \times 10^{-8}$ mol dm^{-3}

Step 3 Substitute them into the equation.

$$[salt] = K_a \times \frac{[acid]}{[H^+(aq)]} = 5.01 \times 10^{-9} \times \frac{0.100}{1.26} \times 10^{-8}$$

$$= 0.0398 \text{ mol dm}^{-3}$$

Step 4 Ask yourself, does this make sense? The pH is lower than the pK_a which means that the concentration of the acid must be greater than that of the conjugate base. Yes, this looks OK!

Question

3 A buffer solution consists of 100 cm^3 of a $0.100 \text{ mol dm}^{-3}$ acid and 50 cm^3 of a solution of its $0.100 \text{ mol dm}^{-3}$ conjugate base (salt). The pK_a of the acid is 4.7. What is the pH of the buffer solution?

Answer

The $K_a = 10^{-pK_a} = 10^{4.7} = 2 \times 10^{-5} \text{ mol dm}^{-3}$

The total volume of the solution = 100 + 50 = 150 cm^3

The concentrations of the acid and the salt or conjugate base have changed when they mix.

The $[acid] = \dfrac{100}{150} \times 0.100 = 0.0667 \text{ mol dm}^{-3}$

The $[salt] = \dfrac{50}{150} \times 0.100 = 0.0333 \text{ mol dm}^{-3}$

$[H^+] = \dfrac{[acid]}{[salt]} \times K_a = \dfrac{0.0667}{0.0333} \times 2 \times 10^{-5} \text{ mol dm}^{-3}$

$= 4 \times 10^{-5} \text{ mol dm}^{-3}$

pH = 4.40. This makes sense because the [acid] is greater than the [salt], so pH should be lower than pK_a value.

Questions

1 Calculate the pH of the following buffer solutions. For each acid you are given the pK_a value and the concentrations of the acid and the salt.

Acid	pK_a	[Acid] / mol dm^{-3}	[Salt] / mol dm^{-3}
a	5.7	0.100	0.075
b	4.1	0.05	0.075
c	8.2	0.105	0.210
d	3.5	0.033	0.050

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.... (*8 marks*)

2 In the following buffer solutions, calculate the pH, the pK_a, the concentration of the acid, or the concentration of the salt as indicated in the table.

Buffer solution	pH of buffer	pK_a of acid	[Acid] / mol dm^{-3}	[Salt] / mol dm^{-3}
a	7.20	7.20	0.100	Calculate
b	4.70	5.10	Calculate	0.05
c	Calculate	6.35	0.100	0.200
d	5.65	Calculate	0.100	0.066

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3 Each of these buffer solutions is made by mixing the given volumes and concentration or weak acid and salt. Calculate the pH of the buffer solution formed.

Buffer solution	pK_a of acid	Volume of acid solution / cm^3	[Acid] / mol dm^{-3}	Volume of salt solution / cm^3	[Salt] / mol dm^{-3}
a	5.00	100	0.100	100	0.150
b	4.2	25	0.200	50	0.150
c	3.5	80	0.050	40	0.075
d	7.2	100	0.066	50	0.050

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Maths skills links to other areas

The use of logarithms is linked to calculations of the activation energy of a reaction using the Arrhenius equation. Rearranging equations comes into many topics including calculation of the rate constant from rate equations.

Answers

1 **a** $K_a = 2.00 \times 10^{-6}$ (*1 mark*); $[H^+] = 2.66 \times 10^{-6}$ (*1 mark*); pH = 5.58

 b $K_a = 7.94 \times 10^{-5}$ (*1 mark*); $[H^+] = 5.30 \times 10^{-5}$ (*1 mark*); pH = 4.28

 c $K_a = 6.31 \times 10^{-9}$ (*1 mark*); $[H^+] = 3.15 \times 10^{-9}$ (*1 mark*); pH = 8.50

 d $K_a = 3.16 \times 10^{-4}$ (*1 mark*); $[H^+] = 2.09 \times 10^{-9}$ (*1 mark*); pH = 3.70 (1 decimal place)   (*8 marks*)

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2 a $[H^+] = 10^{-7.2} = 6.31 \times 10^{-8}$ (*1 mark*); $K_a = 6.31 \times 10^{-8}$; (*1 mark*) [salt] = 0.100 mol dm^{-3}

b $[acid] = \dfrac{[H^+][A^-]}{[K_a]}$; (*1 mark*) $[H^+] = 2 \times 10^{-5}$ mol dm^{-3}; $K_a = 7.94 \times 10^{-6}$ mol dm^{-3}; (*1 mark*)

[acid] = 0.126 mol dm^{-3}; (*1 mark*)

c $K_a = 4.47 \times 10^{-7}$ mol dm^{-3}; (*1 mark*) $[H^+] = 2.24 \times 10^{-7}$ mol dm^{-3}; (*1 mark*) pH = 6.70 (*1 mark*)

d $[H^+] = 2.24 \times 10^{-6}$ mol dm^{-3}; (*1 mark*) $K_a = 1.48 \times 10^{-6}$ mol dm^{-3}; pK_a = 5.83   (*9 marks*)

3 a $K_a = 1 \times 10^{-5}$ mol dm^{-3} (*1 mark*); [acid] = 0.05 mol dm^{-3} (*1 mark*); [salt] = 0.075 mol dm^{-3} (*1 mark*); $[H^+] = 6.67 \times 10^{-6}$ mol dm^{-3} (*1 mark*); pH = 5.17 (*1 mark*)

b $K_a = 6.31 \times 10^{-5}$ mol dm^{-3} (*1 mark*); [acid] = 0.0667 mol dm^{-3} (*1 mark*); [salt] = 0.100 mol dm^{-3} (*1 mark*); $[H^+] = 4.21 \times 10^{-5}$ mol dm^{-3} (*1 mark*); pH = 4.38 (*1 mark*)

c $K_a = 3.16 \times 10^{-4}$ mol dm^{-3} (*1 mark*); [acid] = 0.0333 mol dm^{-3} (*1 mark*); [salt] = 0.025 mol dm^{-3} (*1 mark*); $[H^+] = 4.21 \times 10^{-4}$ mol dm^{-3} (*1 mark*); pH = 3.38 (*1 mark*)

d $K_a = 6.31 \times 10^{-8}$ mol dm^{-3} (*1 mark*); [acid] = 0.0444 mol dm^{-3} (*1 mark*); [salt] = 0.0167 mol dm^{-3} (*1 mark*); $[H^+] = 1.67 \times 10^{-7}$ mol dm^{-3} (*1 mark*); pH = 6.78 (*1 mark*)

(*20 marks*)