Mathematical skills

Maths crops up frequently in GCE chemistry. The weighting for the assessment of mathematical skills is a minimum of 20% but the actual percentage of questions featuring numerical work will be more like 30%. Therefore, it is very important that you feel comfortable answering mathematical questions.

This is an aid to help you master the mathematical skills required in chemistry. Hopefully, it will help you know what to do in many situations. It's been split into five sections.

1. Calculations
2. Equations / formulae
3. Rearranging equations / formulae
4. Changing units
5. Practice questions

1. Calculations

Unfortunately, you can't escape these pesky calculations, but you can get more marks more easily if you follow these rules.

Show your working

This is the most important thing to remember. It could stop you from making silly mistakes and losing out on easy marks. You won't get a mark for a wrong answer, but you could get marks for the method used. Marks will be allocated for individual steps, not just the final answer.

Use correct units

Always give units with your answer – 1g is very different from 1kg!
Converting units is dealt with later but sometimes you'll need to calculate a unit e.g. for an equilibrium constant, K_c.

To work out a unit, substitute the units that you already know into the expression, then cancel out units wherever possible.

Example

For the reaction $2NH_3 \rightleftharpoons N_2 + 3H_2$

$K_c = \frac{[N_2][H_2]^3}{[NH_3]^2}$ Units of $K_c = \frac{(\mathrm{mol\ dm^{-3}})\ (\mathrm{mol\ dm^{-3}})^3}{(\mathrm{mol\ dm^{-3}})^2}$

Cancel $(\mathrm{mol\ dm^{-3}})^2$ from the top and bottom

Units of $K_c = (\mathrm{mol\ dm^{-3}})\ (\mathrm{mol\ dm^{-3}}) = \mathrm{mol^2\ dm^{-6}}$

Use standard form

This makes dealing with very large or very small numbers manageable.

a number between 1 and 10 → $A \times 10^n$ ← the number of places the decimal point moves

Make sure you know how to use standard form on your calculator!

To change a number from decimal to standard form

- Write the non-zero digits with a decimal point after the first digit (this is your integer, A)
- Count how many places you need to move the decimal point until it is directly to the right of the first digit (this is your index number, n)
- If the original number was a decimal, your index number is negative

Example

101000 in standard form

Write the non-zero digits with a decimal point after the first digit ⇨ 1.01

Count how many places you need to move the decimal point until it is directly to the right of the first digit

1 0 1 0 0 0

The decimal point must be moved 5 times ⇨ standard form is 1.01×10^5

To change standard form to decimal

- Move the decimal point n places to the right if n is positive and n places to the left if n is negative
- Fill the gaps with zeros

Example

6.23×10^{-4} in decimal form

n is negative, so move the decimal point 4 places to the left and fill the gaps with zeros

0 0 0 6.2 3

The decimal form is 0.000623

Use significant figures

You should usually consider significant figures rather than decimal places.

Often when you do a calculation, your answer will have many more figures than you need. Using an appropriate number of significant figures will help you to interpret results in a meaningful way.

Remember that

- The first significant figure is the first figure that is not zero
- Zeros that come after the first significant figure count
- Round up the final significant figure if the next figure is 5 or above

Use the number of significant figures given in the data as a guide for how many you need in the answer. Aim to give your answer to the lowest number of significant figures given in the question. However, if you're really unsure round it to three significant figures … unless it's titration data which should be four.

If there are numerous steps in a calculation remember the NAUTE rule – no approximation until the end!

Examples

73.047008 to **four** significant figures is 73.05

0.0000847267 to **three** significant figures is 0.0000847 (or 8.47×10^{-5})

Use tried and tested methods

(a) The method for calculating empirical formulae and water of crystallisation is the same. There are three steps.

Step 1 Find the amount in moles of each element/compound present (divide by M_r)

Step 2 Find the ratio of the number of atoms present (divide by the smallest value in step 1)

Step 3 Convert these numbers into whole numbers (atoms combine in whole number ratios)

To calculate molecular formulae an extra step is needed.

molecular formula = (empirical formula)$_n$ where $n = \frac{M_r \text{ molecular formula}}{M_r \text{ empirical formula}}$

Examples

Calculating empirical and molecular formula

A compound has a relative molecular mass of 88. The percentage composition by mass is C 54.5%; H 9.80%; O 36.4%.

Calculate the empirical formula and the molecular formula.

Step 1
Moles of each element C : H : O

$$\frac{54.5}{12} \quad \frac{9.10}{1.01} \quad \frac{36.4}{16}$$

⇨ 4.54 : 9.01 : 2.275

Step 2
Divide by smallest number ⇨ 2 4 1

Step 3
Empirical formula is C_2H_4O

Empirical formula M_r = 44.04

Number of C_2H_4O units in a molecule = $\frac{88}{44.04}$ = 2

Molecular formula is $C_4H_8O_2$

Calculating water of crystallisation

A 2.15 g sample of $NiSO_4.xH_2O$ was heated to remove the water of crystallisation. After cooling and reweighing it was found that 1.27 g of the anhydrous salt remained. Calculate the value of x in the formula $NiSO_4.xH_2O$.

Step 1
Moles of $NiSO_4 = \frac{1.27}{154.8} = 8.20 \times 10^{-3}$

Mass of $H_2O = 2.15 - 1.27 = 0.88$

Moles of $H_2O = \frac{0.88}{18.02} = 4.88 \times 10^{-2}$

Step 2
Mole ratio of $NiSO_4 : H_2O$

⇨ $8.20 \times 10^{-3} : 4.88 \times 10^{-2}$

Divide by smaller number ⇨ 1 5.95

Step 3
Value of $x = 6$ ⇨ formula is $NiSO_4.6H_2O$

(b) The method for calculating reacting quantities is the same for calculating masses of solids, concentrations of acids or bases and volumes of gases (or percentage purity).

For a reaction aA + bB → cC + dD where you're given information about A and are required to find information about B, the basic method again has three steps.

Step 1 Find the number of moles of A (the substance for which you know the mass, concentration or volume)
Step 2 Use the balanced equation to find the mole (stoichiometric) ratio between A and B, so deduce the number of moles of B
Step 3 Change the number of moles of B to mass, concentration or volume
(If percentage purity is required an extra step is needed)

Examples

Calculating minimum mass

10.0 cm^3 of hydrochloric acid of concentration 2.00 mol dm^{-3} reacts with calcium carbonate.

$$CaCO_3(s) + 2HCl(aq) \rightarrow CaCl_2(aq) + CO_2(g) + H_2O(l)$$

Calculate the minimum mass of calcium carbonate needed to react completely with this amount of acid.

Step 1 Moles of HCl = $\frac{2.00 \times 10}{1000} = 0.0200$

Step 2 Moles of $CaCO_3$ = 0.0100

Step 3 Mass of $CaCO_3$ = $0.0100 \times 100.1 = 1.01$ g

Acid-base titration

A student is given an impure sample of anhydrous sodium carbonate and she carries out an experiment to determine its purity.

She needs 18.0 cm^3 of hydrochloric acid of concentration 0.500 mol dm^{-3} to react completely with 0.550 g of the impure sample. The impurity does not react with hydrochloric acid.

$$Na_2CO_3 + 2HCl \rightarrow 2NaCl + H_2O + CO_2$$

Calculate the mass of sodium carbonate in the sample and hence its purity.

Step 1 Moles of HCl = $\frac{0.500 \times 18.0}{1000} = 9.00 \times 10^{-3}$

Step 2 Moles of Na_2CO_3 = 4.50×10^{-3}

Step 3 Mass of Na_2CO_3 = $4.50 \times 10^{-3} \times 106 = 0.477$ g

Extra step
Percentage purity = $\frac{0.477}{0.550} \times 100 = 86.7$ %

2. Equations / formulae

These are equations that you'll need to **learn** for AS and recall and use in A2 papers too

Amount of substance

number of particles = number of moles × Avogadro constant

The value of the Avogadro constant, N_A, is given in the Data Booklet

For **solids**

number of moles = $\frac{\text{mass of substance}}{\text{relative formula mass}}$ $\qquad n = \frac{m}{M_r}$

For **solutions**

number of moles = $\frac{\text{concentration (mol dm}^{-3}\text{)} \times \text{volume (cm}^3\text{)}}{1000}$

number of moles = $\text{concentration (mol dm}^{-3}\text{)} \times \text{volume (dm}^3\text{)}$ $\qquad n = cV$

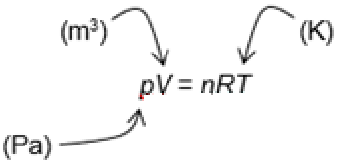
For **gases**

number of moles = $\frac{\text{volume (dm}^3\text{)}}{\text{molar gas volume (dm}^3\text{)}}$ $\qquad n = \frac{V}{V_\text{m}}$

This is only used if pressure is 1 atm and temperature is 273 K (0°C) or 298 K (25°C)

The value of the molar gas volume, V_m, at both of these temperatures is given in the Data Booklet

For an ideal gas



The value of the molar gas constant, R, is in given in the Data Booklet

To measure the volume or pressure of a gas at different temperatures use

$$\frac{p_1V_1}{T_1} = \frac{p_2V_2}{T_2}$$

where values 1 are those at initial conditions and values 2 are those at final conditions

temperatures T_1 and T_2 must be in kelvin, K

Efficiency of a reaction

Percentage atom economy = $\dfrac{\text{total } M_r \text{ of the desired product}}{\text{total } M_r \text{ of the reactants}} \times 100$

Percentage yield = $\dfrac{\textit{actual mass (or moles) of product obtained}}{\textit{theoretical mass (or moles) of product}} \times 100$

Acids

pH = $-\log[H^+]$

$[H^+] = 10^{-pH}$

On most calculators use the following sequence | shift | log | (–) | pH value | =

Equilibrium

For a reaction aA + bB $\rightleftharpoons$ cC +dD

$$K_c = \frac{[C]^c[D]^d}{[A]^a[B]^b}$$

where [C] is concentration of C in mol dm^{-3}
and c is number of moles of C … and so on

Energy changes

To calculate the energy change when a particle absorbs light of a certain frequency use

$$\underset{\text{(J)}}{\Delta E} = h\underset{(\text{Hz or s}^{-1})}{f}$$

$$f = \frac{c}{\underset{\text{(m)}}{\lambda}}$$

where c is the speed of light in m s^{-1} and
where λ is wavelength in metres

To find ionisation energy in kJ mol^{-1} use

ionisation energy = $\Delta E \times N_A$

The values of Planck constant, *h*, speed of light, *c*, and Avogadro's constant, N_A, are given in the Data Booklet

To calculate an enthalpy change of reaction from theoretical data use

enthalpy change of reaction = total energy required to break bonds (reactants) – total energy released in forming bonds (products)

$\Delta H = \Sigma$ (bonds broken) – Σ (bonds formed)

or $\Delta H = \Delta_c H$ (reactants) – $\Delta_c H$ (products)

or $\Delta H = \Delta_f H$ (products) – $\Delta_f H$ (reactants)

To calculate a standard enthalpy change of reaction from experimental data use

heat lost or gained during reaction = mass of solution × specific heat capacity × temperature change

$$\underset{\text{(J)}}{q} = \overset{\text{(g)}}{m}c\,\overset{\text{(K or °C)}}{\Delta T}$$

followed by

$$\underset{(\text{kJ mol}^{-1})}{\Delta H} = \frac{-q}{\underset{\text{(mol)}}{n}}$$

n is the number of moles that has reacted i.e. the number of moles of the substance not in excess

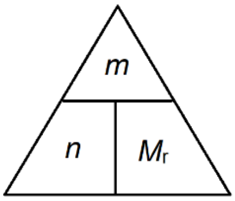
The value of the specific heat capacity of water is given in the Data Booklet

3. Rearranging equations / formulae

This is an essential part of chemistry. You’ll often need to rearrange an equation to make the component that you’ve been asked for the subject of the equation. Always remember whatever you do to one side of the equation you must do to the other side.

Formula triangles are good tools for rearranging an equation if three things are related. The component that is divided goes on the top and the components that are multiplied together go on the bottom. Cover up the component that you’ve been asked for and write down what’s left.

Example



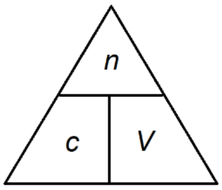
$n = \frac{m}{M_r}$ m is being divided so it goes on the top

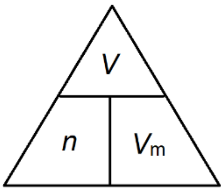
If you want to find the mass cover up ‘m’ leaving ‘$n \times M_r$’

⇨ $m = n \times M_r$

You can also use formula triangles for

$n = c \times V$ and $n = \frac{V}{V_m}$





You can't use a formula triangle to rearrange the equation in the following two examples.

Finding the number of moles of an ideal gas

The equation is $pV = nRT$

If you need to make 'n' the subject of the equation

nRT means n × RT therefore to get n on its own divide by RT

Since you're dividing the right-hand side of the equation by RT you also need to divide the left-hand side by RT

$$\frac{pV}{RT} = \frac{nRT}{RT}$$

Cancel out RT on the right-hand side to leave

$$\frac{pV}{RT} = n$$

Finding the concentration of a component in an equilibrium

For the equilibrium $H_2(g) + Cl_2(g) \rightleftharpoons 2HCl$

$$K_c = \frac{[\mathrm{HCl}]^2}{[\mathrm{H_2}][\mathrm{Cl_2}]}$$

To find the concentration of HCl you need to make '[HCl]' the subject of the equation

To get [HCl] on its own multiply by $[H_2][Cl_2]$

Since you're multiplying the right-hand side of the equation by $[H_2][Cl_2]$ you also need to multiply the left-hand side by $[H_2][Cl_2]$

$$K_c \times [\mathrm{H_2}][\mathrm{Cl_2}] = \frac{[\mathrm{HCl}]^2 \times [\mathrm{H_2}][\mathrm{Cl_2}]}{[\mathrm{H_2}][\mathrm{Cl_2}]}$$

Cancel out $[H_2][Cl_2]$ on the right-hand side to leave

$$K_c \times [\mathrm{H_2}][\mathrm{Cl_2}] = [\mathrm{HCl}]^2$$

Take square roots of both sides to leave

$$\surd(K_c \times [\mathrm{H_2}][\mathrm{Cl_2}]) = [\mathrm{HCl}]$$

4. Changing units

To keep numbers more manageable, we use different units for small and large quantities. The following unit conversions are given in the Data Booklet.

Mass	1 tonne = 1000 kg
Temperature	(˚C) + 273 = K
Pressure	1 atm = 1.01×10^5 Pa
Volume	1 m^3 = 1000 dm^3
	1 dm^3 = 1000 cm^3

Since 1 dm^3 = 1000 cm^3 to get from dm^3 to cm^3 you have to multiply by 1000 (1×10^3) and to get from cm^3 to dm^3 you have to divide by 1000 (1×10^3) which is the same as multiplying by 1×10^{-3}.

$$\begin{tikzcd}
cm^3 \arrow[r, bend left, "\div 1000"] \arrow[rr, bend left=60, "\div 1000000 \text{ or } (\times 10^{-6})"] & dm^3 \arrow[l, bend left, "\times 1000"] \arrow[r, bend left, "\div 1000"] & m^3 \arrow[l, bend left, "\times 1000"] \arrow[ll, bend left=60, "\times 1000000 \text{ or } (\times 10^{6})"]
\end{tikzcd}$$

Similarly

for mass

$$\begin{tikzcd}
g \arrow[r, bend left, "\div 1000"] & kg \arrow[l, bend left, "\times 1000"]
\end{tikzcd}$$

for energy

$$\begin{tikzcd}
J \arrow[r, bend left, "\div 1000"] & kJ \arrow[l, bend left, "\times 1000"]
\end{tikzcd}$$

for pressure

$$\begin{tikzcd}
Pa \arrow[r, bend left, "\div 1000"] & kPa \arrow[l, bend left, "\times 1000"]
\end{tikzcd}$$

Another common change is from nm to m

$$\begin{tikzcd}
nm \arrow[r, bend left, "\div 10^9 \text{ (or } \times 10^{-9})"] & m \arrow[l, bend left, "\times 10^9"]
\end{tikzcd}$$

5. Practice questions

There is no substitute for work. Practise as many questions as you can. Here are some to help you!

1. (a) Convert the following numbers into standard form.

   (i) 4386 (ii) 0.000326 (iii) 58476.3

   (b) Convert the following into decimal form.

   (i) 5.67×10^{-3} (ii) 1.123×10^{4}

2. (a) Write 0.002056543 to **four** significant figures.

   (b) Write 55647 to **three** significant figures.

3. For the reaction $CO_2(g) + H_2(g) \rightleftharpoons CO(g) + H_2O(g)$

   $K_c = \frac{[CO][H_2O]}{[CO_2][H_2]}$

   Give the unit for K_c.

4. For the reaction $CO(g) + 3H_2(g) \rightleftharpoons CH_4(g) + H_2O(g)$

   $K_c = \frac{[CH_4][H_2O]}{[CO][H_2]^3}$

   Give the unit for K_c.

5. 35.7 g of NaCl dissolves in 100 cm^3 of water at 25°C. Calculate the concentration of NaCl in mol dm^{-3}.

6. The solubility of KNO_3 is 133 mg/ml at 0°C. Calculate the concentration of KNO_3 in mol dm^{-3}.

7. 0.115 g of a gas occupies 56 cm^3 at 0°C and 1 atm. Calculate the molar mass of the gas.

8. In an experiment carried out at 30°C and 101 kPa, 245 cm^3 of hydrogen was produced. Calculate the amount, in moles, of hydrogen produced.

9. Nitric acid can be manufactured from ammonia. The first step in the process involves the oxidation of ammonia to nitrogen oxide.

   $4NH_3 + 5O_2 \rightarrow 4NO + 6H_2O$

   (a) Calculate the atom economy for this reaction.

   (b) During this process 255 tonnes of ammonia were oxidised and 260 tonnes of nitrogen oxide produced. Calculate the percentage yield for this reaction.

10. (a) The hydrogen ion concentration of a sample of rainwater was 2.51×10^{-6} mol dm^{-3}. Calculate the pH of the sample.

(b) A sample of orange juice has a pH of 3.82. Calculate the hydrogen ion concentration of this sample.

11. The flame colour for sodium corresponds to a wavelength of 589 nm. Calculate the energy released, in kJ mol^{-1}, when this colour is observed.

12. Consider the equilibrium $2SO_2(g) + O_2(g) \rightleftharpoons 2SO_3(g)$

At a certain temperature the value of the equilibrium constant, K_c, is 316. At this temperature, the equilibrium concentration of SO_3 is 251 mol dm^{-3} and that of SO_2 is 8.4 mol dm^{-3}. Calculate the equilibrium concentration of O_2.

13. Hydrogen can be produced by reforming natural gas.

$$2CH_4 \rightarrow C_2H_4 + 2H_2$$

Use the values in the table below to calculate the enthalpy change for this reaction.

Bond	Average bond enthalpy / kJ mol^{-1}
C – C	348
C = C	612
C – H	412
H – H	436

14. The equation for the reaction between hydrazine and nitrogen dioxide is as follows.

$$2N_2H_4(l) + 2NO_2(g) \rightarrow 3N_2(g) + 4H_2O(l) \qquad \Delta H = -1313 \text{ kJ mol}^{-1}$$

Using this value and the standard enthalpy changes of formation, $\Delta_f H^\theta$, given below, calculate the standard enthalpy change of formation of NO_2.

Substance	$\Delta_f H^\theta$ / kJ mol^{-1}
$N_2H_4(l)$	50.4
$N_2(g)$	0
$H_2O(l)$	–286

15. Magnesium reacts with copper(II) sulfate solution in a displacement reaction.

$$Mg(s) + CuSO_4(aq) \rightarrow MgSO_4(aq) + Cu(s)$$

0.850 g of magnesium was added to 50.0 cm^3 of 0.600 mol dm^{-3} copper(II) sulfate solution in a polystyrene cup. The temperature increased by 10.2°C.

(a) Calculate the energy released in the experiment.

(b) Calculate the molar enthalpy change for the reaction, in kJ mol^{-1}. Give your answer to an **appropriate** number of significant figures.

16. An organic compound contains carbon, hydrogen and oxygen only. It contains 58.8% carbon and 9.8% hydrogen by mass and its relative molecular mass is 102. Calculate both the empirical and molecular formula of the compound.

17. Calcium sulfate can exist as an anhydrous salt or as a hydrated salt, $CaSO_4.xH_2O$. In an experiment to determine the extent of hydration, a 1.91 g sample of hydrated calcium sulfate, $CaSO_4.xH_2O$, was heated to remove all water of crystallisation. The solid remaining had a mass of 1.51 g.

Calculate the value of x in the formula $CaSO_4.xH_2O$.

18. Iron is produced from iron(III) oxide in the blast furnace.

$$2Fe_2O_3(s) + 3C(s) \rightarrow 3CO_2(g) + 4Fe(s)$$

Calculate the maximum mass of iron, in kg, that can be obtained if an excess of carbon and 70 tonnes of iron(III) oxide are used.

19. Barium hydroxide reacts with hydrochloric acid.

$$Ba(OH)_2 + 2HCl \rightarrow BaCl_2 + H_2O$$

A 0.145 g sample of barium hydroxide reacted exactly with 17.00 cm^3 of hydrochloric acid. Calculate the concentration, in mol dm^{-3}, of the hydrochloric acid.

You’ll tackle all the above calculations at AS but you’ll still need them in year 13.

You’ll also learn a few more for your A2 work.

Electrochemical cells

EMF = $E^{\theta}_{\text{reduction}} - E^{\theta}_{\text{oxidation}}$ (positive value means reaction is feasible)

Rates of reaction

for the reaction $\quad A + B \rightarrow \text{products}$

rate = $k\,[A]^m\,[B]^n$

where m is the order of reaction with respect to A, n is the order with respect to B and the overall order is (m + n)

Arrhenius equation

$$k = Ae^{\frac{-\overset{(\text{J mol}^{-1})}{E_a}}{R\underset{(\text{K})}{T}}}$$

unit of rate constant, k = unit of frequency factor, A

Gibbs’ free energy

$$\underset{(\text{kJ mol}^{-1})}{\Delta G} = \overset{(\text{kJ mol}^{-1})}{\Delta H} - \overset{(\text{K})}{T}\underset{(\text{J mol}^{-1})}{\Delta S}$$

Equilibrium

for an equilibrium $aA(g) + bB(g) \rightleftharpoons cC(g) + dD(g)$

$K_p = \frac{p_C{}^c \ p_D{}^d}{p_A{}^a \ p_B{}^b}$ where p_A is partial pressure of A
and a is number of moles of A … and so on

Acid dissociation constants

for an equilibrium $HA(aq) \rightleftharpoons H^+(aq) + A^-(aq)$

$K_a = \frac{[H^+]\,[A^-]}{[HA]}$ unit of K_a is always mol dm^{-3}

for a weak acid, $[H^+] = [A^-]$ therefore

$$K_a = \frac{[H^+]^2}{[HA]}$$

in a buffer solution, $[H^+]$ is not equal to $[A^-]$ since $[A^-]$ = [salt] therefore

$$K_a = \frac{[H^+]\,[\text{salt}]}{[HA]}$$

if [salt] = [HA] ⇨ $K_a = [H^+]$

since $pK_a = -\log(K_a)$ ⇨ $pK_a = pH$

Water

for the equilibrium $H_2O(l) \rightleftharpoons H^+(aq) + OH^-(aq)$

$K_w = [H^+]\,[OH^-]$ unit of K_w is always $mol^2\ dm^{-6}$
the value of K_w is in the **Data Booklet**

You'll also need to be able to rearrange equations such as the following.

Finding a rate constant

for the reaction $C_2H_5Br + OH^- \rightarrow C_2H_5OH + Br^-$

$$\text{rate} = k\,[C_2H_5Br]\,[OH^-]$$

to get the rate constant, k, on its own divide both sides by $[C_2H_5Br]\,[OH^-]$

$$\frac{\text{rate}}{[C_2H_5Br]\,[OH^-]} = \frac{k\,[C_2H_5Br]\,[OH^-]}{[C_2H_5Br]\,[OH^-]}$$

cancel out $[C_2H_5Br]\,[OH^-]$ on the right-hand side

$$\frac{rate}{[C_2H_5Br]\,[OH^-]} = k$$

Using the Arrhenius equation

$$k = Ae^{\frac{-E_a}{RT}}$$

to find the frequency factor, A, divide both sides by $e^{\frac{-E_a}{RT}}$ and cancel out the right-hand side

$$\frac{k}{e^{\frac{-E_a}{RT}}} = A$$

to find the activation energy, E_a, or the temperature, T, you can use natural logs but this is quite complex

it is easier just to remember the expressions

$$E_a = -RT\ln\left(\frac{k}{A}\right) \qquad \text{and} \qquad T = \frac{E_a}{-R\ln\left(\frac{k}{A}\right)}$$

Finding the pH of a weak acid

to find pH you must first find a value for $[H^+]$

for a weak acid $K_a = \frac{[H^+]\,[A^-]}{[HA]}$ and since $[H^+] = [A^-]$

$$K_a = \frac{[H^+]^2}{[HA]}$$

multiply both sides by [HA] and cancel out right-hand side

$$K_a [HA] = [H^+]^2$$

take square root of both sides to get $[H^+]$ on its own

$$\sqrt{}K_a [HA] = [H^+]$$

finally use the equation $pH = -\log [H^+]$