CALCULATIONS FOR IB CHEMISTRY

Created by Mr Field

INTRODUCTION

- The purpose of this presentation, is to collect all the calculations you need for IB Chemistry in one place.
- This will help you to memorise them, but it will NOT help you to master them…the only shortcut to mastery is many hours of dedicated practice.
- Good luck!

PURPOSE:

CALCULATING A QUANTITY IN MOLES FROM A NUMBER OF PARTICLES

The Calculation

$$n = \frac{N}{L}$$

n = the quantity in moles

N = the number of particles

L = Avogadro's constant, 6.02×10^{23}

Notes

- When calculating numbers of atoms within molecules, multiply the number of particles (N) by the number of atoms in the formula
- To find out numbers of particles, rearrange to: $N = n.L$

PURPOSE:
DETERMINE RELATIVE MOLECULAR OR FORMULA MASS, M_R

The Calculation

$$M_r = \sum (number\ of\ atoms.atomic\ mass)$$

Notes

- M_r has no unit as it is a relative value
- To calculate molar mass, M_m, just stick a ‘g’ for grams on the end

PURPOSE:

CALCULATE A QUANTITY IN MOLES, FROM A MASS OF A SUBSTANCE

The Calculation

$$n = \frac{m}{M_m}$$

n = the quantity in moles

m = the mass of substance you are given in grams

M_m = the molar mass of the substance

Notes

- To determine the mass of a given number of moles of a substance use:
- $m = M_m . n$
- To determine the molar mass of a given mass of a substance:
- $M_m = \frac{m}{n}$

STOICHIOMETRY

PURPOSE:
DETERMINE EMPIRICAL FORMULA FROM % COMPOSITION BY MASS

The Calculation

1. Divide each % by the atomic mass
2. Divide each answer to Step 1 by the smallest answer to Step 1
3. Multiply all answers to Step 1 to remove any obvious fractions
   a. If there is a '.5' multiply everything by 2
   b. If there is a '.33' multiply everything by 3 etc

Notes

- You can follow the same method if you have plain composition by mass rather than % composition by mass.

PURPOSE:
DETERMINE MOLECULAR FORMULA FROM EMPIRICAL FORMULA

The Calculation

$$F_m = \frac{M_r}{m(F_e)} . F_e$$

F_m = molecular formula

M_r = relative molecular mass

F_e = empirical formula

$m(F_e)$ = empirical formula mass

Notes

- This and the previous calculation are often combined together in exam questions

PURPOSE:
USE MOLE RATIOS TO DETERMINE THE NUMBER OF MOLES OF 'B' THAT CAN BE MADE FROM 'A'

The Calculation

$$n(B) = n(A)\,.\frac{number\ of\ B\ in\ equation}{number\ of\ A\ in\ equation}$$

Notes

- The second term in this equation is the mole ratio
- You must use a fully balanced equation
- This is the central step in many stoichiometry calculations

STOICHIOMETRY

PURPOSE:
CALCULATE THEORETICAL YIELD

The Calculation	Notes
▪ Use **mole ratios** to determine the expected quantity of product in moles ▪ Use $m = M_m.n$ to determine the expected mass.	▪ n/a

PURPOSE:
DETERMINE LIMITING AND EXCESS REACTANTS

The Calculation

- Divide moles of each reactant by their coefficient in the balanced equation
  - Smallest value = limiting
  - Largest value = excess

Notes

- You would often then need to use mole ratios to determine a quantity of product (in moles).

PURPOSE:
CALCULATING PERCENTAGE YIELD.

The Calculation

$$\%\,Yield = \frac{actual\ yield}{theoretical\ yield} . 100$$

Notes

- Actual and theoretical yield must have the same units.
- You might sometimes be required to rearrange this equation, or use it to work backwards from this to find the amount of reactant you started with.

PURPOSE:
APPLY AVOGADRO'S LAW TO CALCULATE REACTING VOLUMES OF GASES

The Calculation

$$\frac{V_1}{n_1} = \frac{V_2}{n_2}$$

V_1 = the initial volume of gas

n_1 = the initial quantity of gas in moles

V_2 = the final volume of gas

n_2 = the final volume of gas in moles

Notes

- Only applies when temperature and pressure remain constant.
- Units of V do not matter. But must be the same.
- This is really a special case of the Ideal Gas Law where the pressure, temperature and gas constant terms cancel each other out.

PURPOSE:
CALCULATE MOLAR QUANTITIES OF GASES AT STANDARD TEMPERATURE AND PRESSURE

The Calculation

$$n = \frac{V}{22.4}$$

n = quantity in moles

V = the volume of gas in dm^3

22.4 is the molar volume of an ideal gas at 273K and 101,000 Pa

Notes

- Only applies at standard conditions:
  - 273 K (0°C)
  - 101,000 Pa (1.00 atm)
- If volume of gas is given in m^3, use 2.24×10^{-5} as your molar volume.
- Molar volumes are given in the data booklet and do not need memorising.

STOICHIOMETRY

PURPOSE:
THE IDEAL GAS EQUATION

The Calculation

$$PV = nRT$$

P = pressure in Pa

V = volume of gas in m3

n = quantity of gas in moles

R = the gas constant, 8.31

T = temperature in Kelvin (^{O}C + 273)

Notes

- In practice, you can often use:
  - V in units of dm^3
  - Pa in units of kPa
- You will need to be comfortable rearranging this equation to change the subject.
- This takes time to use, so only use it in non-standard conditions, or when the laws in **Calculation 13** would not be quicker.

PURPOSE:

RELATIONSHIP BETWEEN TEMPERATURE, PRESSURE AND VOLUME

The Calculation

Charles' Law, at fixed pressure: $\frac{V_1}{T_1} = \frac{V_2}{T_2}$

Gay-Lussac's Law, at fixed volume: $\frac{P_1}{T_1} = \frac{P_2}{T_2}$

Boyle's Law, at fixed temperature: $P_1V_1 = P_2V_2$

V_1 and V_2 are initial and final volume

P_1 and P_2 are initial and final pressure

T_1 and T_2 are initial and final temperature

Notes

- These only work where the quantity in moles remains fixed.
- All of these are just special cases of the ideal gas law, where the remaining terms just cancel each other out.

PURPOSE:
MOLAR CONCENTRATION

The Calculation

$$c = \frac{n}{V}$$

c = concentration in mol dm^{-3}

n = the quantity in moles

V = the volume in dm^3 (litres)

Notes

- Units are pronounced 'moles per decimetre cubed'
- You need to be able to use any rearrangement of this equation

PURPOSE:
CONCENTRATION BY MASS

The Calculation

$$c = \frac{m}{V}$$

c = concentration in g dm^{-3}

m = the quantity in grams

V = the volume in dm^3 (litres)

Notes

- Units are pronounced ‘grams per decimetre cubed’
- You need to be able to use any rearrangement of this equation
- Generally, if you have a concentration like this, you should convert it into a molar concentration before proceeding.

PURPOSE:
DETERMINE RELATIVE ATOMIC MASS FROM % ABUNDANCE DATA

The Calculation

$$A_r = \sum (atomic\ mass . \frac{\%\ abundance}{100})$$

A_r = relative atomic mass

Notes

- % abundance may be given in the question, or you may need to read it from a mass spectrum
- If you convert the percentages to decimals (i.e. 0.8 for 80%, 0.25 for 25%), there is no need to divide by 100.

PURPOSE:

DETERMINE % ABUNDANCE FROM RELATIVE ATOMIC MASS

The Calculation

If there are two isotopes, label one of them ‘a’ and one ‘b’.

Now: $A_r = \frac{xI_a + yI_b}{x+y}$

However, since x+y = 100%, y = 100-x so:

$$A_r = \frac{xI_a + (100-x)I_b}{100}$$

A_r = relative atomic mass

I_a = the mass of isotope a

I_b = the abundance of isotope b

x and y is the abundance of each isotope

Notes

- A_r, I_a and I_b will be provided in the question, so you can plug the numbers in, and then rearrange to find x.
- To find y, simply do y=100-x
- If you have three isotopes, you must know the abundance of at least one in order to find the other two. You would also need to subtract the abundance of this one from the 100, before doing the rest of the sum.

PURPOSE:

CALCULATING THE HEAT CHANGE OF A PURE SUBSTANCE

The Calculation

$$q = mc\Delta T$$

q = the heat change in Joules

m = the mass of substance in grams

c = specific heat capacity in J K^{-1} g^{-1}

ΔT = temperature rise in K or ^{O}C

Notes

- Be careful of the units of mass…you may need to convert kg into g
- Be careful of the units for specific heat capacity, if it is J K^{-1} kg^{-1} you will need to convert your mass into kg.

PURPOSE:
CALCULATING AN ENTHALPY CHANGE FROM EXPERIMENTAL DATA

The Calculation

$$\Delta H = -mc\Delta T$$

ΔH = the enthalpy change in Joules

m = the mass of solution in grams

c = specific heat capacity of water: 4.18 J K^{-1} g^{-1}

ΔT = temperature rise in K or ^{O}C

Notes

- The minus sign is needed to ensure that an exothermic reaction has a negative enthalpy change.
- Units are J or kJ mol^{-1}
- The mass of solution is assumed to be the same as its volume in cm^3.
- The specific heat capacity of the reactants is ignored.

PURPOSE:
CALCULATING ΔH_R USING A HESS CYCLE

The Calculation

Once you have produced you Hess cycle:

1. Write the relevant ΔH onto each arrow
2. Multiply each ΔH in accordance with the stoichiometry
3. To do your sum, add when you go with an arrow, and subtract when you go against one.

Notes

- See the ‘Energetics’ PowerPoint for advice on constructing Hess cycles.

PURPOSE:

CALCULATING ΔH_R FROM AVERAGE BOND ENTHALPIES

The Calculation

Method 1: Make a Hess cycle, then do as in Calculation 20.

Method 2:

$$\Delta H_r = \sum(reactant\ bonds) - \sum(product\ bonds)$$

Notes

- It is more reliable to use Hess cycles and you can easily forget whether it is reactants – products or vice versa.
- Average bond enthalpies can be found in Table 10 of the data booklet.
- You only need to worry about the bonds that broken and made. If a bond, for example a C-H is present at the start and finish, you can ignore it….this can save time in exams.

HL ONLY

PURPOSE:
CALCULATING ΔH_R FROM ENTHALPIES OF FORMATION

The Calculation

Method 1: Make a Hess cycle, then do as in Calculation 20.

Method 2:

$$\Delta H_r = \sum \Delta H_f^{\theta}(products) - \sum \Delta H_f^{\theta}(reactants)$$

ΔH_r = enthalpy change of reaction

$\Delta H^{\ominus}_f$ = enthalpy change of formation

Notes

- It is more reliable to use Hess cycles and you can easily forget whether it is products – reactants or vice versa.
- $\Delta H^{\ominus}_f$ for elements in their standard states is zero.
- $\Delta H^{\ominus}_f$ values for many compounds can be found in Table 11 of the data booklet.
- In some questions, you may also need to take a state change into account, if standard states are not used.

PURPOSE:

CALCULATING ΔH_R FROM ENTHALPIES OF COMBUSTION

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The Calculation

Method 1: Make a Hess cycle, then do as in Calculation 20.

Method 2:

$$\Delta H_r = \sum \Delta H_c^{\theta}(reactants) - \sum \Delta H_c^{\theta}(products)$$

ΔH_r = enthalpy change of reaction

ΔH°_c = enthalpy change of combustion

Notes

- It is more reliable to use Hess cycles and you can easily forget whether it is reactants – products or vice versa.
- ΔH°_c for CO_2 and H_2O is zero.
- ΔH°_c values for many compounds can be found in Table 12 of the data booklet.

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PURPOSE:
CALCULATING LATTICE ENTHALPY

The Calculation	**Notes**
You need to build a Born-Haber cycle….see the Energetics PowerPoint for help.	- n/a

ENERGETICS

PURPOSE:

CALCULATING ΔS FROM STANDARD ENTROPY VALUES

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The Calculation

$$\Delta S^{\theta} = \sum S^{\theta}(products) - \sum S^{\theta}(products)$$

$\Delta S^{\ominus}$ = standard entropy change of reaction

$S^{\ominus}$ = standard entropy of each substance

Notes

- Units are J K^{-1} mol^{-1}
- $S^{\ominus}$ values can be found in Table 11 of the data booklet
- You cannot assume that $S^{\ominus}$ of an element is zero. It is not.

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PURPOSE:

CALCULATING ΔG STANDARD GIBBS' FREE ENERGY OF FORMATION VALUES

The Calculation

Method 1: Make a Hess cycle, then do similar to Calculation 20.

Method 2:

$$\Delta G_r = \sum \Delta G_f^{\theta}(products) - \sum \Delta G_f^{\theta}(reactants)$$

ΔG_r = Gibb's free energy of reaction

$\Delta G^{\ominus}_f$ = Gibb's free energy of formation

Notes

- Units are J or kJ mol^{-1}
- It is more reliable to use Hess cycles and you can easily forget whether it is products – reactants or vice versa.
- $\Delta G^{\ominus}_f$ for elements in their standard states is zero.
- $\Delta G^{\ominus}_f$ values for many compounds can be found in Table 11 of the data booklet.

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PURPOSE:
CALCULATING ΔG FROM EXPERIMENTAL DATA

The Calculation

$$\Delta G = \Delta H - T\Delta S$$

ΔG = Gibb's free energy

ΔH = Enthalpy change

T = Temperature in Kelvin

ΔS = Entropy change

Notes

- If ΔH is in kJ mol^{-1}, you will need to divide ΔS by 1000 to convert it to units of kJ K^{-1} mol^{-1}
- You may first need to calculate ΔH and ΔS using **Calculations 23** and **24**.

PURPOSE:
CALCULATE THE RATE OF A REACTION

The Calculation

$$Rate = \frac{-\Delta[R]}{\Delta t} = \frac{\Delta[P]}{\Delta t}$$

Δ[R] = change in reactant concentration

Δ[P] = change in product concentration

Δt = change in time

Notes

- Units are mol dm^{-3} s^{-1}
- The minus sign in front of Δ[R] is because the concentration of reactants decreases

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PURPOSE:
CALCULATE THE GRADIENT OF A SLOPE

The Calculation

$$Gradient = \frac{change\ in\ y}{change\ in\ x}$$

Notes

- Used for calculating rate from graph of concentration (y-axis) over time (x-axis)

PURPOSE:

DETERMINE THE ORDER OF REACTION WITH RESPECT TO A REACTANT, X.

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The Calculation

1. Identify two experiments, where the concentration of ‘x’ has changed, but all others have remained the same.
2. Compare the change in [x] to the change in rate:
   a. If doubling [x] has no effect on rate, then 0th order.
   b. If doubling [x] doubles rate, then 1st order.
3. If doubling [x] quadruples rate, then 2nd order.

Notes

- Sometimes, you can’t find two cases where only [x] has changed, in which case you may need to take into account the order of reaction with respect to other reactants.

HL ONLY

PURPOSE:
DEDUCE A RATE EXPRESSION

The Calculation

$$Rate = k[A]^x[B]^y[C]^z$$

k = rate constant (see below)

[A/B/C] = concentration of each reactant

x/y/z = order of reaction with respect to each reactant

Notes

- Reactants with a reaction order of zero can be omitted from the rate equation
- Given suitable information, you may need to calculate the value of the rate constant if given rates, concentrations and reaction order, or the expected rate given the other information.

HL ONLY

PURPOSE:
DETERMINING THE UNITS FOR THE RATE CONSTANT

The Calculation

$$Units = \frac{mol\ dm^{-3} s^{-1}}{mol^{x}(dm^{-3})^{x}}$$

- mol and dm^{-3} terms on the top and the bottom should be cancelled out
- Remaining mol and dm^{-3} terms on the bottom should then be brought to the top by inverting their indices.

x = the overall order of the reaction

Notes

- If you can't understand this, try to memorise:
  - 0th order: mol dm^{-3} s^{-1}
  - 1st order: s^{-1}
  - 2nd order: mol^{-1} dm^{3} s^{-1}
  - 3rd order: mol^{-2} dm^{6} s^{-1}

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PURPOSE:
DETERMINING ACTIVATION ENERGY

The Calculation

- The Arrhenius equation: $k = Ae^{\frac{-E_a}{RT}}$
- This rearranges to: $\ln k = \frac{-E_a}{R} . \frac{1}{T} + \ln A$
- Which is basically the equation for a straight line in the form ‘y=mx+c’ where: ‘y’ is ln k; ‘x’ is 1/T; ‘m’ is –E_a/R; ‘c’ is ln A
- So, if we do a reaction at a range of temperatures and calculate ln k, then:

1. Draw a graph with 1/T along the x-axis, and ln k on the y-axis
2. Draw a straight line of best fit.
3. Determine the gradient of the line
4. Then: $E_a = -Gradient \times R$

Notes

- Where:
  - k = rate constant
  - A = Arrhenius constant
  - e = exponential constant
  - Ea = activation energy
  - R = gas constant, 8.31
  - T = temperature in Kelvin
- Units of E_a are kJ mol^{-1}
- From the graph, you might also be asked to calculate A:
  - ‘ln A’, is the y-intercept of the graph, so simply raise ‘e’ to the power of this intercept.

KINETICS

PURPOSE:
DETERMINING THE EQUILIBRIUM CONSTANT EXPRESSION

The Calculation

For the reaction:

wA + zB → yC + zD

$$K_c = \frac{[C]^y[D]^z}{[A]^w[B]^z}$$

K_c = equilibrium constant

Notes

- Only applies to reactants for which there is a concentration:
  - Aqueous substances are included
  - Solids and pure liquids are omitted as they do not have a concentration per se
- For reactions involving gases, use partial pressures instead of concentrations.
- At SL, you only need be able to construct the expression.
- At HL, you may need to calculate K_c from the expression and suitable data, or to determine reactant equilibrium concentrations of reactants, given K_c and suitable information.

PURPOSE:

DETERMINING CHANGES IN [H^+] GIVEN CHANGES IN PH

The Calculation

- For each increase of '1' on the pH scale, divide [H^+] by 10.
- For each decrease of '1' on the pH scale, multiply [H^+] by 10

Notes

- At SL, you do not need to be able to calculate pH, just to understand it in relative terms.

PURPOSE:
DEDUCE [H$^+$] AND [OH$^-$] GIVEN K$_W$

The Calculation

$$K_w = [H^+].[OH^-]$$

So:

$$[H^+] = \frac{K_w}{[OH^-]}$$

And:

$$[OH^-] = \frac{K_w}{[H^+]}$$

Notes

- At standard conditions, $K_w = 1.00\text{x}10^{-14}$
- Kw varies with temperature, so it is important to know how to do this calculation.

PURPOSE:
CALCULATING PH FROM $[H^+]$ AND VICE VERSA

The Calculation

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

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

Notes

- With strong acids, you can assume $[H^+]$ is the same as the concentration of the acid (adjusted for the stoichiometry)
- With weak acids, you will need to calculate $[H^+]$ using K_a or pK_a.

HL ONLY

PURPOSE:

CALCULATING PH FROM [OH$^-$] AND VICE VERSA

The Calculation

$$pOH = -log_{10}[OH^-]$$

$$[OH^-] = 10^{-pOH}$$

Notes

- With strong bases, you can assume [OH$^-$] is the same as the concentration of the acid (adjusted for the stoichiometry)
- With weak acids, you will need to calculate [OH$^-$] using K_b or pK_b.

HL ONLY

PURPOSE:

DETERMINING K_A AND K_B OF ACIDS/BASES AND THEIR CONJUGATE BASES/ACIDS

The Calculation

$$K_w = K_a . K_b$$

So:

$$K_a = \frac{K_w}{K_b}$$

And:

$$K_b = \frac{K_w}{K_a}$$

Notes

- This is useful when trying of determine the strength the conjugate base of a weak acid, and the conjugate acid of a weak base.

HL ONLY

PURPOSE:

DETERMINING PK$_A$ AND PK$_B$ OF ACIDS/BASES AND THEIR CONJUGATE BASES/ACIDS

The Calculation

$$pK_w = pK_a + pK_b$$

So:

$$pK_a = pK_w - pK_b$$

And:

$$pK_b = pK_w - pK_a$$

Notes

- This is useful when trying of determine the strength the conjugate base of a weak acid, and the conjugate acid of a weak base.

PURPOSE:

DETERMINING PH FROM POH AND VICE VERSA

HL ONLY

The Calculation

$$pK_w = pK_a + pK_b$$

So:

$$pH = 14 - pOH$$

And:

$$pOH = 14 - pH$$

Notes

- This is useful to quickly and easily calculate one of pH/pOH from the other (or $[H^+]$/$[OH^-]$).

HL ONLY

PURPOSE:

CALCULATING PH OF A SOLUTION OF A WEAK ACID

The Calculation

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

Since [H$^+$] = [A$^-$]: $K_a = \frac{[H^+]^2}{[HA]}$

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

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

Notes

- We assume that [HA] is equal to the concentration stated in the question, as only a very small amount has dissociated.
- You may need to work backwards from pH to work out K$_a$:

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

- Then: $K_a = \frac{[H^+]^2}{[HA]}$
- You will not need to work out problems for polyprotic weak acids that would require quadratics.

ACIDS AND BASES

HL ONLY

PURPOSE:

CALCULATING POH OF A SOLUTION OF A WEAK BASE

The Calculation

$$K_b = \frac{[B^+][OH^-]}{[BOH]}$$

Since [B$^+$] = [OH$^-$]:

$$K_b = \frac{[OH^-]^2}{[BOH]}$$

So:

$$[OH^-] = \sqrt{K_b.[BOH]}$$

Then:

$$pOH = -log_{10}[OH^-]$$

Notes

- We assume that [BOH] is equal to the concentration stated in the question, as only a very small amount has dissociated.
- You may need to work backwards from pOH to work out K_b:

$$[OH^-] = 10^{-pOH}$$

- Then:

$$K_b = \frac{[OH^-]^2}{[BOH]}$$

ACIDS AND BASES

PURPOSE:

DETERMINING PH OF ACIDIC BUFFER SOLUTIONS (AND ALKALI BUFFERS)

HL ONLY

The Calculation

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

Now $[H^+]$ is not equal to $[A^-]$:

So:

$$[H^+] = \frac{K_a.[A^-]}{[HA]}$$

Then:

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

Notes

- You may need to use your stoichiometry to calculate the [HA] and [A-] in the buffer solution first.
- Since additional A^- is added, we now need to use the concentration of A^- from the buffer as our $[A^-]$.
- [HA] should either be that stated in the question, or that calculated via stoichiometry, depending on the context.
- For alkali buffers, do the same process but with OH^-, K_b etc.

HL ONLY

PURPOSE:

CALCULATE $E^{\ominus}_{CELL}$

The Calculation

$$E^{\theta}_{cell} = E^{\theta}(cathode) - E^{\theta}(\text{anode})$$

$E^{\ominus}_{cell}$ = cell potential

$E^{\ominus}$ = standard electrode potential

Notes

- The value should always be positive, so if you get it the wrong way round, just take off the minus sign.
- $E^{\ominus}$ can be found in the data booklet.
- You do not need to take the stoichiometry of the reaction into account, just use the $E^{\ominus}$as they are in the data booklet.

PURPOSE:

CALCULATING RELATIVE UNCERTAINTIES (IN %)

The Calculation

$$\text{Relative uncertainty} = \frac{\text{absolute uncertainty}}{\text{size of value}}.100$$

Notes

- Large measurements have lower relative uncertainties

PURPOSE:
CALCULATING ABSOLUTE UNCERTAINTY WHEN ADDITION/SUBTRACTION IS INVOLVED

The Calculation

$$Total\ uncertainty = \sum (absolute\ uncertainties)$$

Notes

- This only works when adding and subtracting values with the same units

PURPOSE:
CALCULATING RELATIVE UNCERTAINTY WHEN MULTIPLICATION/DIVISION IS INVOLVED

The Calculation

$$Total\, uncertainty = \sum (relative\, uncertainties)$$

Notes

- For use when you are multiplying/dividing values with different units

PURPOSE:
CALCULATING THE ENERGY VALUE OF FOOD FROM COMBUSTION DATA

The Calculation

Use:

$$q = mc\Delta T$$

q = the heat change in Joules

m = the mass of substance in grams

c = specific heat capacity in J K^{-1} g^{-1}

ΔT = temperature rise in K or ^{O}C

Notes

- You may need to convert the energy value into a value per mole by dividing q by the number of moles of substance burnt.

PURPOSE:
CALCULATING IODINE NUMBERS

The Calculation

- $N(I_2) = m(I_2).\frac{100}{m(lipid)}$
-
- $N(I_2)$ = the iodine number
- $m(I_2)$ = the mass of iodine reacting in g
- m(lipid) = the mass of lipid involved in g

Notes

- All units should be grams
- You may need to convert from data involving bromine to an ‘iodine equivalent’…just use your stoichiometry

PURPOSE:

CALCULATE THE NUMBER OF DOUBLE BONDS IN A LIPID USING IODINE NUMBER.

The Calculation

Calculate the quantity in moles of I_2 corresponding to the iodine number:

$$n(I_2) = \frac{N(I_2)}{M_r(I_2)}$$

Calculate the quantity in moles of lipid in 100g:

$$n(lipid) = \frac{100}{M_r(lipid)}$$

Then the number of double bonds is:

$$Double\ bonds = \frac{n(I_2)}{n(lipid)}$$

Notes

$N(I_2)$ = the iodine number

n = quantities in moles

M_m = molar masses

- This works because each mole of double bonds reacts with one mole of iodine.