I B Chemistry Investigations

Volume 1 (Standard Level)

COPY MASTERS

(For use with the IB Diploma programme)

(Fourth edition)

Author: John Green

Series editor: David Greig

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Name _____ *Date* _____ *Teacher* _____

The object of this Investigation is to provide practice in calorimetric techniques by measuring the heat evolved or absorbed in both a physical and a chemical change.

In these experiments you will need to calculate the heat gained or lost using the equation:

Heat change = mass × specific heat × temperature change

The heat changes will be those used to heat/cool the water or aqueous solution and to a first approximation you may ignore the heat gained or lost by the polystyrene calorimeter and the other substances present. Another useful approximation is to assume that, like water, dilute aqueous solutions have a density of 1 kg dm^{-3} and a specific heat capacity of 4.18 kJ dm^{-3} K^{-1}.

Part A – The heat required for a change of state

METHOD

1) By mixing hot and cold water in a measuring cylinder, put 100 cm^3 of water at about 60°C into a polystyrene cup.

2) Dry about 25 g of ice with a piece of paper towel, weigh them both and record the mass.

3) Rapidly record the temperature of the water, transfer the ice to it, then record the mass of the paper towel and the water it has absorbed.

4) Stir the water-ice mixture and record the temperature of the water as soon as all the ice has just melted.

DATA COLLECTION

Mass of ice, paper towel and water = _____ ± _____ g

Mass of paper towel and water   = _____ ± _____ g

Initial temperature of water   = _____ ± _____ °C

Final temperature of water   = _____ ± _____ °C

Volume of water   = _____ ± _____ cm^3

Relevant qualitative data

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DATA ANALYSIS

a) Calculate the heat lost by the warm water.

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b) Calculate the heat gained to raise the temperature of the molten ice to the final temperature.

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c)   Use these data to calculate the heat required to melt the ice.

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d)   From this result, calculate the latent heat of fusion of ice in kJ mol^{-1}.

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e)   Use your values for the precision of the readings to calculate the uncertainty of the latent heat of fusion.

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Part B – Determining the enthalpy change for the decomposition of aqueous hydrogen peroxide

METHOD

1)   Take a polystyrene cup and use a measuring cylinder to put 50 cm^3 of 2 mol dm^{-3} aqueous hydrogen peroxide into it.

2)   Weigh out about 1 g of manganese(IV) oxide into a weighing bottle.

3)   Stir and record the temperature of the hydrogen peroxide at half minute intervals for 2 minutes and then add the manganese(IV) oxide.

4)   Stir the mixture and record the temperature at half minute intervals until the temperature has been falling for ten consecutive readings.

DATA COLLECTION

Time /s	Temperature /°C	Time /s	Temperature /°C	Time /s	Temperature /°C
0		210		420	
30		240		450	
60		270		480	
90		300		510	
120		330		540	
150		360		570	
180		390		600	

Precision of time measurements   ± _____ s

Precision of temperature measurements   ± _____ °C

Volume of aqueous hydrogen peroxide   = _____ ± _____ cm³

Relevant qualitative data

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DATA ANALYSIS

Plot a graph of temperature against time and draw the best straight line through the initial section and the final cooling section. You may use a spreadsheet or a graph-plotting programme for this, or you may prefer to hand-draw the graph.

a)   Use this graph to estimate the rise in temperature that would have occurred if the reaction had been instantaneous and heat had not been lost to the environment. Explain what assumptions you are making in estimating this.

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b)   Calculate the heat energy produced by the reaction.

c)   From the amount (in mol) of hydrogen peroxide calculate the enthalpy change when 1 mol undergoes decomposition

d)   Write a balanced equation for the reaction and calculate ΔH for your equation.

CONCLUSION & EVALUATION

a)   Look up the accepted value for the enthalpy of fusion of ice and compare it to the value you have determined, taking into account the uncertainty. What does this imply?

b)   The enthalpy of formation of hydrogen peroxide is -187.8 kJ mol^{-1}. Use this value, along with other relevant values from your data booklet, to calculate the expected enthalpy change for the reaction.

c)   Use your data booklet to find bond enthalpy values for the bonds that are broken and made during the reaction. Use these data to calculate a second value for the expected enthalpy of reaction.

d)   Which of these values would you expect to be the more accurate? Give your reasons.

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e)   Using the value you consider to be the more accurate prediction, comment on the accuracy of your result taking into account the uncertainty.

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f)   What assumptions have been made in these determinations? Are these likely to be able to explain the accuracy of the results obtained?

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g)   What are the major sources of error in these calorimetry experiments? Is the direction of the systematic errors in keeping with the direction of the deviation of the experimental results?

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h)   Suggest ways in which the accuracy of either, or both, of the determinations could be significantly improved.

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TEACHING NOTES

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Contents with Syllabus references

No.	Title	Topic	Syllabus reference
1A	Determining the Water of Crystallisation	1.2	Obtaining and using experimental data for deriving empirical formulas from reactions involving mass changes.
1B	Determining the Composition of "Copper Carbonate"	1.2	
1C	How Concentrated is "Concentrated" Nitric Acid?	1.3	Use of the experimental method of titration to calculate the concentration of a solution by reference to a standard solution
1D	Determining the Molar Mass of a Soluble Acid	1.3	
1E	Identifying fuels from their molar masses	1.3	Obtaining and using experimental values to calculate the molar mass of a gas from the ideal gas equation.
2A	Observing Emission Spectra	2.2	Emission spectra could be observed using discharge tubes of different gases and a spectroscope. Flame tests could be used to study spectra.
3A	Some Reactions of the Halogens	3.2	Experiment with chemical trends directly in the laboratory or through the use of teacher demonstrations.
4A	Forces Between Particles and Physical Properties	4.1	Students could investigate compounds based on their bond type and properties.
5A	Measuring Enthalpy Changes	5.1	A calorimetry experiment for an enthalpy of reaction should be covered and the results evaluated. Experiments could include calculating enthalpy changes from given experimental data (energy content of food, enthalpy of melting of ice or the enthalpy change of simple reactions in aqueous solution).
5B	Using Hess' Law to Determine Enthalpy Changes	5.2	A calorimetry experiment for an enthalpy of reaction should be covered and the results evaluated. Experiments could include Hess's Law labs.
6A	Techniques for Measuring Reaction Rates	6.1	Investigation of rates of reaction experimentally and evaluation of the results. Experiments could include investigating rates by changing concentration of a reactant or temperature.
6B	Factors Affecting Rates of Chemical Reactions	6.1	Investigation of rates of reaction experimentally and evaluation of the results. Experiments could include investigating rates by changing concentration of a reactant or temperature.
6C	A Quantitative Investigation of Reaction Rates	6.1	Investigation of rates of reaction experimentally and evaluation of the results. Experiments could include investigating rates by changing concentration of a reactant or temperature.
7A	An Introduction to Equilibrium	7.1	The characteristics of chemical and physical systems in a state of equilibrium. Physical and chemical systems should be covered.
7B	An Introduction to Vapour Pressure	7.1	The characteristics of chemical and physical systems in a state of equilibrium. Physical and chemical systems should be covered.
7C	Predicting the Effect of Changes on an Equilibrium	7.1	Le Châtelier's principle can be investigated qualitatively by looking at pressure, concentration and temperature changes on different equilibrium systems.
8A	The Solubility of Ethanedioic (Oxalic) Acid	8.2	Candidates should have experience of acid-base titrations with different Indicators. The evidence for these properties could be based on a student's experimental experiences.
8B	Percentage of Nitrogen Content in a Fertilizer	8.2	Candidates should have experience of acid-base titrations with different Indicators. The evidence for these properties could be based on a student's experimental experiences.

No.	Title	Topic	Syllabus reference
8C	A Comparison of Strong and Weak Acids and Bases	8.4	Students should be familiar with the use of a pH meter and universal indicator. Students should have experimental experience of working qualitatively with both strong and weak acids and bases. Examples to include: H_2SO_4 (aq), HCl (aq), HNO_3 (aq), NaOH (aq), NH_3 (aq).
9A	Common Oxidizing and Reducing Agents	9.1	Experiments could include demonstrating the activity series, redox titrations and using the Winkler Method to measure BOD.
9B	Redox Titrations	9.1	Experiments could include demonstrating the activity series, redox titrations and using the Winkler Method to measure BOD.
9C	Investigating some Electrochemical Cells	9.2	Performance of laboratory experiments involving a typical voltaic cell using two metal/metal-ion half-cells.
10A	Investigating Organic Structures using Models	10.1	Construction of 3-D models (real or virtual) of organic molecules.
10B	Reactions of Hydrocarbons	10.2	Experiments could include distinguishing between alkanes and alkenes.
10C	Reactions of Organic Compounds containing Oxygen	10.2	Experiments could include reflux and distillation.
11A	Analysis of Organic Spectra	11.3	Deduction of information about the structural features of a compound from percentage composition data, MS, ^{1}H NMR or IR.
OPTION TOPICS			
22A	Investigating the Behaviour of Catalysts	A.3	Experiments could include investigating the decomposition of potassium sodium tartrate with cobalt chloride and the decomposition of hydrogen peroxide with manganese (IV) oxide.
23A	The Chromatographic Separation of Amino acids	B.2	Experiments could involve identification of amino acid mixtures by paper chromatography.
24A	The Enthalpy of Combustion of fuels	C.1	The energy density of different fuels could be investigated experimentally.
25A	The Synthesis of Aspirin	D.2	Experiments could include the synthesis of aspirin.

Key to Required Practicals

No.	Topic	Requirement
1	Topic 1.2	Determination of the molecular formula of a compound from its empirical formula and molar mass.
2	Topic 1.3	Obtaining and using experimental values to calculate the molar mass of a gas from the ideal gas equation.
3	Topic 1.3	Use of the experimental method of titration to calculate the concentration of a solution by reference to a standard solution
4	Topic 5.1	A calorimetry experiment for an enthalpy of reaction should be covered and the results evaluated.
5	Topic 6.1	Investigation of rates of reaction experimentally and evaluation of the results.
6	Topic 9.2	Performance of laboratory experiments involving a typical voltaic cell using two metal/metal-ion half-cells.
7	Topic 10.1	Construction of 3-D models (real or virtual) of organic molecules.
8	Topic 15.1 / Topic 19.1	Perform lab experiments which could include single replacement reactions in aqueous solutions.

SYLLABUS RELEVANCE: TOPIC 5.1

A calorimetry experiment for an enthalpy of reaction should be covered and the results evaluated.

Experiments could include calculating enthalpy changes from given experimental data (energy content of food, enthalpy of melting of ice or the enthalpy change of simple reactions in aqueous solution).

Apparatus required

Per group

- Thermometer (0–110ºC)
- Stop watch
- 100 cm³ measuring cylinder
- Weighing bottle
- Polystyrene cup
- Electric stirrer

Generally available

- Balance capable of weighing to at least 0.01 g
- Paper towels
- Kettle(s)

Chemicals required

- Ice (~25 g per group)
- Aqueous 2 mol dm^{-3} hydrogen peroxide (~50 cm³ per group)
- Powdered manganese(IV) oxide (manganese dioxide, ~1 g per group)

Notes

Probable timing–60 minutes laboratory time

A fairly straightforward thermochemistry practical that gives reasonably good results, though the latent heat generally gives better results than the enthalpy of reaction and there are less embarrassing questions about whether one should take into account the specific heat of manganese(IV) oxide.

Part A

Mass of ice, filter paper and water = 31.104 ± 0.0005 g

Mass of filter paper and water = 8.135 ± 0.0005 g

Initial temperature of water = 66.8 ± 0.1 ºC

Final temperature of water = 37.4 ± 0.1 ºC

Volume of water = 100 ± 0.5 cm³

Relevant Qualitative Data

When drying the ice the water absorbed by the towel tends to drip off. Before the ice is added steam is visible rising from the surface of the hot water. When the ice is added to the water the size of the lumps of ice gradually decreases and eventually disappear.

a) $Q = m \cdot c \cdot \Delta T = 100 \times 4.18 \times (66.8 - 37.4) = 12289.2$ J $= 12.29$ kJ

b) $Q = m \cdot c \cdot \Delta T = (31.104 - 8.135) \times 4.18 \times (37.4 - 0) = 3590.8$ J $= 3.59$ kJ

c)   Heat lost by water = Heat required to melt ice + Heat required to heat water after melting

       $12.29 = x + 3.59$

       $x = 12.29 - 3.59 = 8.70$ kJ

d)   22.969 (=31.104 – 8.135) g of ice required 8.70 kJ to melt so 1 mole (18.02 g) would require:

$$8.70 \times \frac{18.02}{22.969} = 6.83 \text{ kJ mol}$$

e)   Use your values for the precision of the readings to calculate the precision of this value

Quantity	Value	Absolute uncertainty	Percentage uncertainty
Volume of water	100	0.5	0.500
Decrease in water temperature	29.4	0.2	0.680
Heat lost by water	12.29	0.145	1.180
Mass of ice	22.969	0.001	0.004
Increase in ice temperature	37.4	0.1	0.267
Heat gained by molten ice	3.59	0.010	0.271
Heat required to melt ice	8.70	0.155	1.782
Molar enthalpy of fusion	6.83	0.122	1.786

Molar enthalpy of fusion of water = 6.8 ±0.1 kJ mol^{-1}

Part B

Time /s	Temperature /°C	Time /s	Temperature /°C	Time /s	Temperature /°C
0	19.0	210	69.0	420	58.5
30	19.0	240	67.0	450	57.5
60	19.0	270	65.0	480	56.0
90	19.0	300	63.5	510	55.0
120	19.0	330	62.0	540	54.5
150	33.0	360	61.0	570	53.0
180	64.0	390	60.0	600	52.5

Precision of time measurements   = ± 1 s

Precision of temperature measurements   = ± 0.25 °C

Volume of aqueous hydrogen peroxide   = 50 ± 0.5 cm³

Relevant qualitative data

Initial very rapid reaction with evolution of gas and a little splashing out of a few droplets. After about a minute this subsided to leave a colourless liquid with black powder in the bottom and adhering to the sides of the container.

Data Analysis
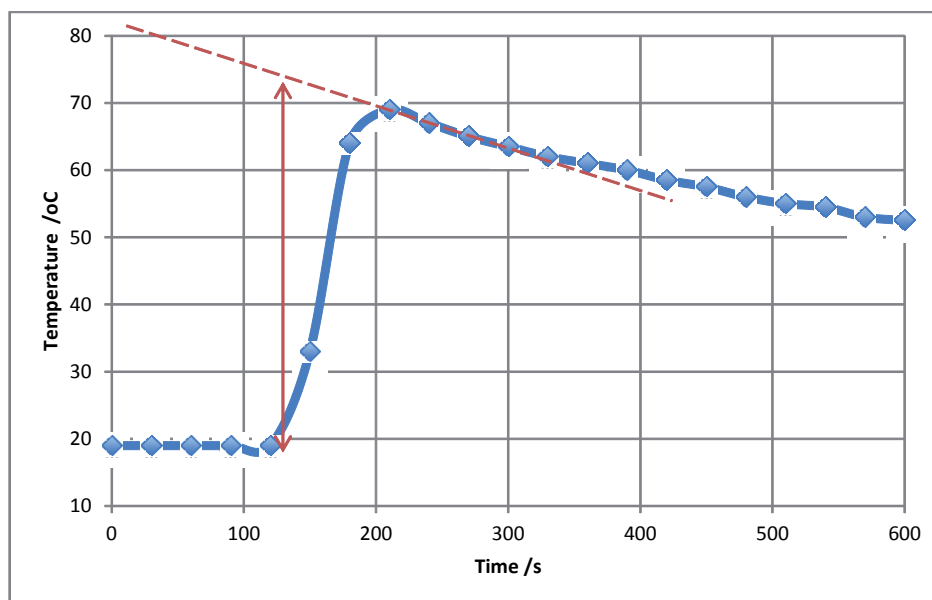
a) Rise in temperature if the reaction was instantaneous and the rate of heat loss was the same as in the initial stages of cooling, is shown on the graph above. It gives a value of:

$\Delta T = 74 - 19 = 55 \pm 1$ °C (uncertainty estimated as accuracy of reading graph)

b) Heat to raise water temp = heat produced by reaction

$Q = m.c.\Delta T = 50 \times 4.18 \times 55 = 11,495$ J = 11.495 kJ

Uncertainty in mass = uncertainty in volume = $\pm 1\%$

Uncertainty in temperature change = 1.8%

Total uncertainty in Q = $\pm 2.8\%$

c) Amount of H_2O_2 = n = c.V = $1.0 \times 0.050 = 0.050$

$\Delta H = \dfrac{Q}{n} = \dfrac{11.495}{0.05} = 229.9\, kJ\, mol^{-1}$

Uncertainty in n = uncertainty in V = $\pm 1\%$

Total uncertainty in ΔH = 3.8% = ± 8.7 kJ

Enthalpy change of reaction:

$2\, H_2O_{2\,(aq)} \rightarrow 2\, H_2O_{(l)} + O_{2\,(g)}$ = -115 ± 9 kJ (negative as reaction is exothermic)

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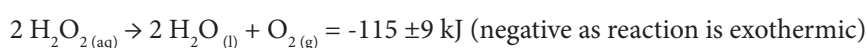
Conclusion & Evaluation

a) The accepted value for the enthalpy of fusion of ice is 6.01 kJ mol^{-1}. This value is less than the values determined (13% lower) and lies well outside the uncertainty of the experimentally determined value, implying that the procedure involves significant systematic errors.

b) $\Delta H = \Sigma \Delta H_f$ (products) $- \Sigma \Delta H_f$ (reactants) $= (2 \times 285.5) - (2 \times 187.8) = -195.4$ kJ mol^{-1}

   (Remember ΔH_f of oxygen = 0, like all elements in their standard states)

c) In the reaction, two O-O single bonds are being replaced by a O=O double bond; the O-H bonds remain the same. Hence

   $\Delta H = (2 \text{ x } +144) - (498) = -210$ kJ mol^{-1}

d) The value derived from standard enthalpies of formation should be the more accurate, the only source of error being that the reaction carried out involved aqueous hydrogen peroxide rather than the pure compound, so enthalpies of solution were neglected. In the case of the bond enthalpies the value for the O-O bond is an average value of all compounds that contain this bond and it may differ from the precise value in hydrogen peroxide. It also assumes that the bond enthalpies of the O-H bonds remain unchanged and this is probably not correct as the electronegativity of the atom joined on to the second bond of oxygen will affect its electronegativity and hence the strength of the O-H bond. Finally bond enthalpy data is only really valid for reactions taking place in the gas phase and this was in aqueous solution. For all these reasons, the bond enthalpy value is probably less accurate.

e) As may be expected from a thermochemistry determination in simple apparatus, the experimental value for "uppercase delta"H is considerably less than the theoretical one: 115 kJ mol^{-1} compared to 195 kJ mol^{-1} (~41% too small). The most probable explanations for this is that the graphical extrapolation of the temperature underestimates the heat lost to the surroundings, because during the period of cooling no hot gas is being evolved, a process that was occurring during the reaction.

f) Like all calorimetric techniques these methods both assume that there is no gain or loss of heat to the surroundings. Heat losses are often significant and could easily explain deviations from literature values of the order of magnitude observed. In addition the hydrogen peroxide involves the loss of gas from the apparatus and this would carry heat away.

   This hydrogen peroxide experiment also assumes that the density and specific heat capacity of the aqueous hydrogen peroxide is equal to that of water. In practice the density of the aqueous solution is greater than that of water (~10% higher) and the specific heat capacity of the pure liquid is less (2.62 rather than 4.18 J g^{-1} K^{-1}) so at least the direction of the errors cancel, but the actual values of these two quantities for the solution used should be determined.

g) If heat was lost to the surroundings the final temperature (37.4°C) would be below the true value so the heat lost by the water (12.29 kJ) would be greater than the true value and the heat gained by the molten ice (3.59 kJ) would be less than the true value. Therefore the heat required to melt the ice, and the enthalpy of fusion, would have been overestimated, as was indeed found.

   A second significant source of error in this is that the mass is assumed to be that of ice and no water was transferred to the calorimeter. In practice the ice is always wet, so the true mass of ice is less than the measured mass (22.969 g). This would lead to the value determined for the enthalpy of fusion being smaller than the value determined, which was not what was found, hence it would appear that errors resulting from heat losses are greater than those resulting from the ice being wet.

A third potential source of error is that if the ice has been obtained fresh from the freezer then the centre of the ice will not be at 0°C, but will be at a lower temperature. As a result the heat needed to raise the temperature of the ice to its melting point needs to be added to the equation. This would mean the enthalpy of fusion was greater than the true value as was observed.

h) The loss of heat to the surroundings could be reduced by putting the polystyrene cup inside a second polystyrene cup, so as to provide additional insulation and, perhaps even more importantly, a polystyrene lid with a hole for the thermometer could be fitted to the cup.

The dryness of the ice could be improved by ensuring that there is adequate paper towel to absorb water from the surface and by minimising the surface area of the ice.

Finally to control the starting temperature the ice to be used could be stored in a beaker immersed in an ice-water bath for sufficient time for the ice to be at 0°C.

Inaccuracies associated with the assumptions about the density and specific heat capacity of aqueous hydrogen peroxide could be removed by actually determining these values experimentally.

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