

D ASSESSING DATA QUALITY: CHEMICAL DATA

This is a lesson aimed at helping students to develop their understanding of how to assess the quality of scientific data.

Resources for students and teachers

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OHT D0.1 Aims of the lesson Activity D1 Cards 1–6 (6 sheets) Teachers' presentation notes D2.1A and B Dealing with uncertainty OHT D2.2 Dealing with uncertainty OHT D2.3A and B Variation of emission rate of a radioactive substance with concentration OHT D2.4 Variation of emission rate of a radioactive source with concentration Sheet D2.5A/B What value to choose? Group task sheets D3.1A–E Sheet D3.2 'Molar heat capacity and entropy of calcium metal' Reprinted from the *Journal of Chemical Thermodynamics* (5 sheets) Sheet D4.1 Dealing with errors in A-level Chemistry practical work Sheet D4.2 Student's report on an experiment to find out how the energy in fuels depends on the structure of the molecules (2 sheets)

Teachers' notes (separate download)

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by Andy Hind, John Leach, and Jim Ryder: University of Leeds Tricia Combe: Ilkley Grammar School

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Aims of the lesson

During this lesson you will develop your understanding in the following areas:

In the first activity:

• the different reasons why scientific measurements always include a degree of uncertainty.

In the second activity:

• the techniques that scientists use to deal with experimental error;

• what error bars tell us about experimental data.

In the final activity

• how the quality of a set of data can be assessed.

ACTIVITY CARD 1 POLLUTION MONITORING

Following an industrial accident, an analytical chemist is measuring the concentration of a pollutant in a lake. Measurements of the concentration of the pollutant are made at various key locations around the lake. At each point where measurements are to be made, several samples of water are taken and the concentration of the pollutant is measured in each sample.

At 12.00 p.m. on the day following the accident, 10 measurements of the concentration of the pollutant were made at one of the key locations around the lake. The values measured for the concentration of the pollutant at this location alone vary between

 $1.09 \times 10^{-4} \text{ mol dm}^{-3}$ and

 $1.23 \text{ x } 10^{-4} \text{ mol dm}^{-3}$.

ACTIVITY CARD 2 RADIO-IMMUNOASSAY

The technique of radio-immunoassay is commonly used in biochemical analysis to trace pathways of chemical reactions in living tissues.

['Radio' suggests that the technique involves the use of radioactivity, 'immuno' suggests that the technique is related to the immune system, 'assay' means 'measuring technique'.]

Radioactive atoms such as ¹³C are attached to molecules called immunoglobulins that bind very specifically to particular proteins in the cell. The location of the radioactive atoms can then be measured.

A biochemist is measuring the amount of radioactive ¹³C that has accumulated in a particular part of the brain. However, in making the measurements he has not taken into account background radiation in the laboratory.

ACTIVITY CARD 3 ISOLATING GENES

A molecular biologist is working to isolate a gene from a thermophilic species of bacteria, using a standard technique.

('Thermophilic' means that the bacteria can survive in much hotter conditions than most species of bacteria.)

However, the isolation has not worked properly because the buffer solution used was contaminated. A different gene has been isolated. The molecular biologist has not yet realised that the technique has not worked.

ACTIVITY CARD 4 MODELLING THE ATMOSPHERE

The atmosphere is very complex. The concentration of gases is different in different layers of the atmosphere. The atmosphere has many currents of air. In order to make predictions about the weather, and long-term changes in the atmosphere such as enhanced global warming, atmospheric chemists have developed various mathematical models of atmospheric processes using computers. These models make predictions based on large amounts of measured data about current atmospheric conditions such as average air temperatures at different latitudes.

Two teams of researchers are using different mathematical models of the atmosphere to make predictions about global warming. Even though each team are putting the same set of measured data into the model, their predictions about global warming are very different.

ACTIVITY CARD 5 RATE OF REACTION

A physical chemist is making measurements of the rate of a reaction. She has repeated the procedure 10 times.

The calculated values for the initial rate of reaction for the formation of one of the products vary between 1.33×10^{-6} and 1.62×10^{-6} mol dm⁻³ s⁻¹.

ACTIVITY CARD 6 TITRATIONS

An analytical chemist is using titration to measure the concentration of a molecule in solution.

A calibration curve has been prepared, which shows the volume required to titrate against various known concentrations of the molecule. Using this method, the concentration of the molecule is calculated very precisely as 0.127 mol dm⁻³.

DEALING WITH UNCERTAINTY

The aim of the presentation is to show students how uncertainty about measurements can be dealt with. The key information to be communicated to the students is highlighted in the boxes.

Dealing with random error

Any measured value includes a degree of uncertainty.

An individual measurement will have random error associated with it. To deal with this, scientists estimate error bars by considering the accuracy of the instrumentation used to make the measurement. For example a measurement of temperature could be reported as 283.4 ± 0.1 K.

If an experimental procedure involves many steps, scientists can use a set of rules to combine individual random errors for the whole process.¹

An alternative way of estimating random error is to repeat the measurements many times to obtain a **set of data**. The spread of the data set can be used to calculate error bars around the mean value.²

¹ The determination of many physical constants such as rate constants and enthalpies of combustion involve large numbers of individual measurements such as solute masses, solution volumes, and changes in temperature. Each of these measurements will introduce its own random error to the experimental procedure. One way of dealing with this is to estimate each individual uncertainty based on the accuracy of instrumentation used to make each measurement, and then use rules of error propagation to estimate the uncertainty in the final value.

² It is felt that for A-level chemistry students it is not necessary to explain the statistical methods used to calculate the error bars (usually 95% confidence limits) for a large data set. In professional science, experimental measurements are repeated many times, a process aided by fast data acquisition technology. However, in their individual experimental work, AS/A-level chemistry students rarely repeat their entire experimental procedure enough times to obtain large data sets, and they are unlikely to need to calculate standard deviations and 95 % confidence limits. AS/A-level Biology and Maths students will come across or may have already covered ideas about normal distributions, standard deviation, and confidence limits, and it may be felt appropriate to discuss exactly how the error bars can be calculated with individual students.

What do error bars tell us?

Error bars give an estimate of the range of likely values for the measurement. The narrower the range, the more precise the estimate.

When plotting a graph of experimental measurements, it is important to plot the error bars.

When plotting a line or curve of best fit, it is important to consider the range of likely values within the error bars not just the central plotted value.

OHT D2.3 shows a set of experimental measurements plotted with error bars. Students should be asked: 'Where should the line of best fit be placed?' Two possible lines of best fit have been provided and each one can be overlaid in turn.

Line A passes through four of the plotted values exactly. However, it should be pointed out that the aim is not to place the line of best fit through the maximum possible number of plotted values, but to fit the line to the plotted ranges depicted by the error bars.

Line B is a better choice as it minimises the distance between the plotted values and the best fit line and also lies within all the plotted ranges.

Often with straight-line graphs, it is the value of the gradient and/or intercept that we are interested in. The uncertainty in a value obtained in this way can be estimated by plotting both the steepest and shallowest possible lines passing through the plotted range for each data point.

OHT D2.4 can be used to illustrate this point. In this case an estimate of the range in which the background radiation lies is given by the difference between the intercepts of the two extreme lines.

Dealing with systematic error

Systematic errors can usually be dealt with by applying a correction factor. Some examples of systematic errors are:

• measurements of radiation emissions from a source where the background radiation has not been corrected for;

• measurements in calorimetry where heat loss to the surroundings has not been corrected for.

Background radiation is a good example to use for the purpose of illustrating systematic error to students. OHT D2.4 shows the concentration of a radioisotope in solution against the counts per minute emitted. Background radiation can be estimated by extrapolating the graph to a concentration of zero. A correction factor can then be applied to the other measurements.

Issues to do with modelling

It is worth pointing out to students that none of the above techniques will show the extent to which the assumptions of models are valid. However precise a measurement is, it is not necessarily the 'true' value. If the assumptions or model used are inappropriate then the estimated value, of whatever precision, may not be accurate. The CODATA disclaimer on sheet D2.5a highlights this.

Dealing with Uncertainty

Example 1 **T = 283.4 ± 0.1 K**

Why has the temperature been reported like this? How has the uncertainty been estimated?

Example 2 What do the crosses tell you about the measurements? What do the bars tell you about the measurements?



Variation of emission rate of a radioactive substance with concentration



To overlay lines A and B, align the index crosses on the extreme left and right of each line (OHT D2.3B).

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Overlay



Variation of emission rate of a radioactive source with concentration



WHAT VALUE TO CHOOSE?

In industry and research, chemists rely on agreed values of certain measurements. This saves them spending time determining information which is already published. In the same way you use values from a data book in your work.

Some scientists are employed to make such measurements as accurately as possible. The Committee on Data for Science and Technology (CODATA) was set up in 1966. The aim of this committee is to improve the quality and reliability of data that is important in science and technology.

One of the roles of CODATA is to publish agreed data on the thermodynamic properties of substances. The values given represent the consensus judgement of an international group of experts and are based on measurements by a number of different scientists.

While they believe there is a high probability that the true values fall within the stated uncertainty limits, CODATA do not assume responsibility for any consequences of the use of these data.

The following is an extract from their published table.

Substance	State	Enthalpy of formation at 298.15 K / kJ mol ⁻¹
calcium	gaseous	177.8 ± 0.8

Task 1

In pairs, discuss the following questions. Your teacher will ask you to feed back your ideas to the rest of the class.

1 What does the figure ± 0.8 tell you about the value for the enthalpy of calcium?

2 Why have CODATA chosen to present the data to four significant figures?

3 Why do you think they include the disclaimer: 'We [CODATA] do not assume responsibility for any consequences of the use of these data.' ?

WHAT VALUE TO CHOOSE? continued

Task 2

The table below presents a set of measurements made by a group of scientists who were employed to work out the molar heat capacity of calcium at 298 K.

Molar heat capacity is a measurement of the amount of energy needed to raise 1 mole of a substance by 1 K.

Twenty measurements have been made. They have been put in order in the table, with the lowest measurement first. The measurements were made on the most sophisticated equipment available, which was very carefully calibrated. Some simple statistics have been calculated for the set of measurements.

The scientists now have to decide what figure to publish as the molar heat capacity of calcium at 298 K.

Molar heat / J K ⁻¹ mol ⁻		Mean (average)	= 25.16
24.98 25.00 25.03 25.05 25.07 25.09 25.10 25.11 25.12 25.13	25.14 25.16 25.17 25.17 25.17 25.19 25.21 25.22 25.24 25.80	Mode (most common value Median (value in the middle the rank-ordered list	= 25.17 e) $= 25.14$ e of t)

In your groups answer the following questions.

1 Some of the experts on the CODATA committee think that the result of 25.80 J K^{-1} mol⁻¹ should not be counted. Do you agree with them? Why?

2 The value 25.17 J K^{-1} mol⁻¹ was measured on three different occasions. Do you think this is significant?

3 What value do you think should be used for the published data tables?

MOLAR HEAT CAPACITY MEASUREMENT: GROUP 1

If you compare the figures published for molar heat capacity in data books over the years, you will see that they change.

In the case of the molar heat capacity for calcium, a group of American scientists from the US Geological Survey felt that, since the published result is based on 60year-old data collected with outdated measurement techniques, the accuracy is questionable. Measurement techniques in this field have improved, so they decided to obtain a more accurate value using the new techniques.

You are provided with an extract of the article they published in the *Journal of Chemical Thermodynamics*. You also have the commentary on the article given below to help you understand it.

Read lines 1-6.

The following notes will help you understand the article.

Lines 1–6

This is the abstract of the article. It gives a very brief summary of the findings of the article to help people decide if it is of use to them. It explains that 85 measurements have been taken of the heat capacity of calcium at different mean temperatures.

It is not necessary to understand the technical details of the method or equipment used.

The figures stated are the values that the authors have concluded from their measurements.

With your partner discuss the following questions. You will be asked to feed back to the class your thoughts on each question.

1 Why do the authors refer to measurements at 'mean temperatures' and not a precise temperature?

2 What is the significance of the range of temperatures being given to approximate values?

MOLAR HEAT CAPACITY MEASUREMENT: GROUP 2

If you compare the figures published for molar heat capacity in data books over the years, you will see that they change.

In the case of the molar heat capacity for calcium, a group of American scientists from the US Geological Survey felt that, since the published result is based on 60year-old data collected with outdated measurement techniques, the accuracy is questionable. Measurement techniques in this field have improved, so they decided to obtain a more accurate value using the new techniques.

You are provided with an extract of the article they published in the *Journal of Chemical Thermodynamics*. You also have the commentary on the article given below to help you understand it.

Read lines 16–25.

The following notes will help you understand the article.

Lines 16-25

The authors have used highly advanced techniques to obtain as pure a sample of calcium as possible. However, even after further purification, the sample will still contain a number of impurities – in this case oxygen, hydrogen, nitrogen, carbon and barium.

With your partner discuss the following questions. You will be asked to feed back to the class your thoughts on each question.

1 Do you think the 'major impurities' (line 21) in the sample will affect the measurements?

2 Can anything be done to counteract the effect?

MOLAR HEAT CAPACITY MEASUREMENT: GROUP 3

If you compare the figures published for molar heat capacity in data books over the years, you will see that they change.

In the case of the molar heat capacity for calcium, a group of American scientists from the US Geological Survey felt that, since the published result is based on 60year-old data collected with outdated measurement techniques, the accuracy is questionable. Measurement techniques in this field have improved, so they decided to obtain a more accurate value using the new techniques.

You are provided with an extract of the article they published in the *Journal of Chemical Thermodynamics*. You also have the commentary on the article given below to help you understand it.

Read lines 50-61.

The following notes will help you understand the article.

Lines 50-61

The final value stated by the authors is not what they measured. They have made a correction to their figures to account for the impurities in the sample. The impurities, oxygen, hydrogen, nitrogen, carbon and barium have different heat capacities and this will affect the accuracy of the measurements. The authors have used a variety of techniques (lines 21–25) to measure the amount of impurity in a sample and used this information in their assumptions about the composition of the samples tested.

The authors have also assumed that there is no calcium hydroxide in the sample.

With your partner discuss the following questions. You will be asked to feed back to the class your thoughts on each question.

1 Refer to lines 50–61. Why did the authors 'assume that 100 g of sample was made up of

99.356 g of Ca, 0.333 g of CaO, 0.250 g of CaH $_2$ etc.'

2 What was this assumption based on? Refer to lines 21–25.

MOLAR HEAT CAPACITY MEASUREMENT: GROUP 4

If you compare the figures published for molar heat capacity in data books over the years, you will see that they change.

In the case of the molar heat capacity for calcium, a group of American scientists from the US Geological Survey felt that, since the published result is based on 60year-old data collected with outdated measurement techniques, the accuracy is questionable. Measurement techniques in this field have improved, so they decided to obtain a more accurate value using the new techniques.

You are provided with an extract of the article they published in the *Journal of Chemical Thermodynamics*. You also have the commentary on the article given below to help you understand it.

Study Table 1. The following notes will help you understand the article.

Table 1

This table presents the measurements of molar heat capacity made over a range of mean temperatures. The measurements are presented in chronological order; the order is not significant. They are not corrected for impurities.

With your partner discuss the following questions. You will be asked to feed back to the class your thoughts on each question.

1. Refer to Table 1. What evidence is there in the table that the results may be precise but are not accurate?

2. Did the authors systematically repeat readings?

3. Do you think repeat readings are necessary in this case?

MOLAR HEAT CAPACITY MEASUREMENT: GROUP 5

If you compare the figures published for molar heat capacity in data books over the years, you will see that they change.

In the case of the molar heat capacity for calcium, a group of American scientists from the US Geological Survey felt that, since the published result is based on 60year-old data collected with outdated measurement techniques, the accuracy is questionable. Measurement techniques in this field have improved, so they decided to obtain a more accurate value using the new techniques.

You are provided with an extract of the article they published in the *Journal of Chemical Thermodynamics*. You also have the commentary on the article given below to help you understand it.

Read lines 62-72.

The following notes will help you understand the article.

Lines 62-72

In order to improve the results the authors have made corrections for the presence of calcium hydride (CaH₂) in the sample. To do this they needed a value for the heat capacity of CaH₂. Since measurements for CaH₂ are only published for a few temperatures, they made an estimate based on other metal hydrides for other temperatures.

They justify this assumption by plotting results for the different metal hydrides, which shows a difference of approximately 6%.

With your partner discuss the following questions.

You will be asked to feed back to the class your thoughts on each question.

Refer to line 62. To make corrections for impurities the authors have made an estimate of the molar heat capacity of each impurity.

- **1** What are the estimates based on?
- **2** Do you think the estimates are valid? Why?

ASSESSING DATA QUALITY: CHEMICAL DATA

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Molar heat capacity and entropy of calcium metal

Bruce S. Hemingway, Richard A. Robie,

U.S. Geological Survey, 959 National Center, Reston, VA 22092, U.S.A. and Malcolm W. Chase (to whom correspondence should be addressed) Physical and Chemical Properties Division, National Institute of Standards and Technology, Gaithersburg, MD 20899, U.S.A.

The heat capacity of calcium has been measured at 85 mean temperatures between $T \approx 8$ K and $T \approx 369$ K using an adiabatically-shielded calorimeter in an intermittent heating mode. At T = 298.15 K, the recommended values for the molar heat capacity, molar entropy, and molar enthalpy increment referred to T = 0 are

 (25.77 ± 0.08) JK⁻¹mol⁻¹, (42.90 ± 0.11) JK⁻¹mol⁻¹, and (5811 ± 12) J mol⁻¹, 5 respectively. The uncertainties are twice the standard deviation of the mean.

KEYWORDS: calcium; calorimetry; entropy; heat capacity; thermodynamic properties

1. Introduction

Although calcium is one of the more common elements (ranking ninth in abundance in 10 the Earth's crust), the thermodynamic data for the pure element, in particular the entropy, are based upon measurements of limited accuracy made more than 60 years ago on samples of questionable purity.

A sample of calcium metal was obtained and purified in anticipation of measuring the low-temperature heat capacity and high-temperature enthalpy. This article presents the 15 results for low-temperature heat capacity.

2. Experimental

The calcium sample was obtained from the Aesar Group, Seabrook, NH.[†] It was classified by them as "Bright crystalline (dendritic) solid, reaction, 99.98 per cent (low oxygen), ampouled under argon". Subsequent chemical analysis showed the sample to contain mass fraction ≈ 0.01 of oxygen. The sample was further purified (distillation) by D. Peterson continued

20 at the Ames Laboratory, Iowa State University.

[†]Any use of trade names in this report is for descriptive purposes only and does not constitute endorsement by the U.S. Geological Survey or the National Institute of Standards and Technology.

The major impurities in the reprocessed calcium sample are: oxygen, mass fraction, 95×10^{-3} (fast neutron activation analysis); hydrogen, mass fraction, 12×10^{-5} (vacuum fusion in molten tin bath); nitrogen, mass fraction, 74×10^{-6} (method not given); carbon, mass fraction, 14×10^{-6} (heating to T = 1573 K in O₂ atmosphere, CO₂ measured by i.r. detector);

- 25 and barium, mass fraction, 4 x 10⁻⁴ (emission spectrography). The sample mass was 13.883 g. The sample was loaded into the calorimeter at the National Institute of Standards and Technology (NIST) in a glovebox under an atmosphere of dry Ar(g) and temporarily sealed. The calorimeter was placed in a desiccator also filled with dry Ar(g), and then transferred to the laboratory at the U.S. Geological Survey (Reston, VA). The calorimeter
- 30 was then unsealed, placed in the vacuum sealing jig, and rapidly evacuated to a pressure p < 10 Pa. It was then backfilled with dry helium gas at p = 5 kPa, and sealed. This sealing procedure effectively kept the calcium metal from exposure to air; however, the sample was not analysed after the heat-capacity measurements were completed.
- The calorimeter, cryostat, and the automation of the data acquisition system used for 35 the measurements have been described. Temperatures were measured with a 100 Ω (R₀) Mincot model S1059-1 strain-free miniature platinum resistance thermometer, which had been calibrated by the Temperature Measurements Section of NIST on IPTS-68 between the temperatures 13.8 K and 505 K. Below T = 13.8 K, temperatures are based on a scale derived from the resistance at the boiling temperature of helium and the NIST calibration,
- 40 together with equations given by McCrackin and Chang. (The conversion to ITS-90 makes no significant difference to the recommended thermal functions due to the uncertainty in the results.)

3. Results

The heat capacity of calcium was measured at 85 mean temperatures between $T \approx 8$ K and $T \approx 369$ K using an automatic, adiabatically-shielded calorimeter in an intermittent heating

- 45 mode. Our experimental results, corrected for curvature but not for the impurities in the sample, are listed in table 1 in their chronological order of measurement, and are shown graphically in figure 1. The contribution of the calcium sample to the total heat capacity measured of (sample + calorimeter) ranged from a maximum of 50 per cent at T = 21 K to a minimum of 23 per cent at T = 369 K.
- 50 For the purpose of correcting our measurements to values for $C_{p,m}^{\circ}$ of pure Ca, we assumed that 100 g of sample was made up of 99.356 g of Ca, 0.333 g of CaO, 0.250 g of CaH₂, 0.0035 g of N₂, 0.014 g of C, and 0.04 g of Ba. For CaO, we have used the $C_{p,m}^{\circ}$ values of Gmelin. For carbon and nitrogen, we used the values tabulated by Hultgren *et al*, and for barium those of Furukawa and Ishihara. The correction for CaH₂ is discussed below.
- 55 The effect of the corrections is fairly small. The difference between the corrected and uncorrected $C_{p,m}^{\circ}$ values for calcium corresponds to $0.5 \times 10^{-2} \times C_{p,m}^{\circ}$ at T = 50 K, $-0.3 \times 10^{-2} \times C_{p,m}^{\circ}$ at T = 100 K, $-0.4 \times 10^{-3} \times C_{p,m}^{\circ}$ at T = 200 K, and $0.8 \times 10^{-3} \times C_{p,m}^{\circ}$ at T = 300 K.

It was assumed that Ca(OH)₂, if originally present in the calcium sample, would have decomposed in the purification (distillation) procedure. However, if all the oxygen were bound as Ca(OH)₂, rather than CaO, the heat capacity correction would be $1 \times 10^{-3} \times C_{p,m}^{\circ}$ at

T = 300 K, instead of $0.8 \times 10^{-3} \times C_{p,m}^{\circ}$.

To make the correction for CaH_2^p we have estimated its $C_{p,m}^{\circ}$. Gunther measured $C_{p,m}^{\circ}$ of CaH_2 between T = 69.9 K and T = 86.2 K and these are apparently the only measurements available. Flotow and Osborne measured $C_{p,m}^{\circ}$ of ZrH_2 and Flotow *et al.* measured $C_{p,m}^{\circ}$ of

65 YH₂ between T = 5 K and T = 350 K. Using the values listed in Hultgren *et al.*, for $C_{p,m}^{\bullet}$ of Zr and Y and the above results for the hydrides, we constructed a graph of $C_{p,m}^{\bullet}$ (metal)/ $C_{p,m}^{\bullet}$ (hydride) for the two hydrides. Between T = 100 K and T = 300 K, both graphs are essentially linear and the ratios have the same values to within ≈ 6 per cent.

From a straight-line plot of the values of $C_{p,m}^{\circ}(M)/C_{p,m}^{\circ}(MH_2)$ (M = Y, Zr) against *T*, 70 together with our results for Ca, the unpublished $C_{p,m}^{\circ}$ of MgH₂, and the limited set of

actual $C_{p,m}^{\circ}$ measurements for CaH₂, we estimated $C_{p,m}^{\circ}$ for CaH₂ between T = 8 K and T = 370 K.

Т	$C^{\circ}_{p,\mathrm{m}}$	Т	$C^{\circ}_{p,\mathrm{m}}$	Т	$C^{\mathbf{o}}_{p,\mathbf{m}}$	
 K	$\frac{1}{\mathbf{J} \mathbf{K}^{-1} \mathbf{mol}^{-1}}$	 K	$\overline{\mathbf{J}\mathbf{K}^{-1}\mathbf{mol}^{-1}}$	 K	$\overline{\mathbf{J}\mathbf{K}^{-1}\mathbf{mol}^{-1}}$	
	Series 1	Serie	s 4	Seri	es 5	
306.56	25.89	296.19	25.89	116.35	21.55	
311.50	25.95	301.42	25.80	121.96	21.88	
		306.63	25.89	127.54	22.19	
Series 2				133.08	22.49	
		Serie	s 5	138.60	22.74	
300.86	25.77			144.10	22.95	
306.01	25.80	8.34	0.0965	149.57	23.15	
311.01	25.94	9.39	0.1508	155.02	23.32	
		10.24	0.1935	160.45	23.46	
	Series 3	11.27	0.2711	165.86	23.61	
		12.56	0.3757	171.26	23.78	
318.10	25.91	13.96	0.5255			
323.19	26.00	15.52	0.7286	Seri	es 6	
328.17	26.14	17.26	1.010			
333.16	26.19	19.17	1.392	176.51	23.93	
338.27	26.21	21.30	1.891	181.84	24.05	
343.40	26.44	23.69	2.533	186.92	24.21	
348.54	26.47	26.36	3.353	192.02	24.32	
353.66	26.49	29.36	4.364	197.21	24.44	
358.78	26.48	32.72	5.590	202.40	24.48	
363.89	26.49	36.50	7.013	207.57	24.60	
368.99	26.56	40.75	8.423	212.74	24.66	
		45.48	10.19	217.90	24.74	
	Series 4	50.72	11.83	223.06	24.87	
		56.62	13.49	228.23	24.94	
249.78	25.11	62.87	14.99	233.42	25.00	
254.44	25.27	69.16	16.26	238.62	25.11	
259.53	25.24	75.39	17.46	243.84	25.11	
264.63	25.34	81.48	18.24	249.08	25.17	
269.93	25.43	87.44	19.01	254.32	25.22	
275.21	25.49	93.34	19.67			
280.48	25.53	99.18	20.26	Seri	es 7	
285.73	25.62	104.97	20.77			
290.97	25.X3	110.69	21.17	300.68	25.80	
				305.73	25.87	

TABLE 1. Experimental molar heat capacities $C_{p,m}^{\circ}$ of calcium corrected for curvature but not for impurities (Molar mass = 40.078 g mol⁻¹)

Figure 1 Experimental molar heat capacities $C_{p,m}^{\circ}/R$ of calcium metal uncorrected for impurities. (Molar mass = 40.078 g mol⁻¹).



End

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DEALING WITH ERRORS IN A-LEVEL CHEMISTRY PRACTICAL WORK

For this assignment, you are presented with the report of an A-level Chemistry student (sheet D4.2). The student was given the task of measuring the amount of energy released when different alcohols are burnt.

The student measured the rise in temperature of a known volume of water when heated for one minute by a burner containing one of four alcohols. In each case the student measured the mass of fuel used.

Knowing the molecular weight of each alcohol and the specific heat capacity of water, the student calculated the energy change during combustion (ΔH_c).

The measurements were carried out three times for each alcohol.

Please read the student's report before you complete the following tasks.

Questions

1 What do the error bars tell you about each set of data?

Questions 2 and 3 ask you to estimate the heat of combustion of a 5-carbon alcohol by extrapolating from the graphs.

2 Draw a line/curve of best fit on to the graph. Explain why you have chosen to draw that particular line.

3 Extrapolate from the graph to make an estimate of the heat of combustion of pentan-1-ol, which has 5 carbon atoms in each molecule.

4 Adding together the bond energies for each bond in the molecule gives a reliable prediction for the heat of combustion. This gives an expected value for ΔH°_{c} for pental-1-ol of -3328 kJ mol⁻¹. Identify as many reasons as you can as to why the estimate made from the graph differs from the expected value based on the bond energy calculation. [Hint: think about errors and assumptions.]

Student's report on an experiment to find out how the energy in fuels depends on the structure of the molecules

My aim in this experiment was to find out if the amount of energy an alcohol gives out when it burns depends on the number of carbon atoms in each molecule.

Method

For my experiment I used a calorimeter because I thought this might give me better results. I set it up like in the diagram.

For each measurement I recorded the temperature before and after I burnt the fuel, and the mass of the burner, before and after to tell me how much fuel I burnt. I did the experiment for 1 minute each time. I stirred the water while I was heating it.

I measured the room temperature and looked up the specific heat capacity of water; the room was at 298 K so the specific heat capacity of water is 4179 J.

I also looked up the mass of 1 mole of each alcohol. I used this information to calculate the energy given out by 1 mole of each alcohol. On my graph I plotted the average of my three measurements with estimated error bars. To work out my error bars, I decided that the largest random error was the measurement of the temperature change. I could measure the temperature to \pm 0.1 °C. This gives an estimated error of about 10%.



Student's report on an experiment to find out how the energy in fuels depends on the structure of the molecules continued

Results

	Reading			
	1	2	3	Average
Methanol	-496.70	-511.31	-613.58	-540.53
Ethanol	-894.46	-983.90	-1001.79	-960.05
Propan-1-ol	-1399.31	-1541.83	-1541.83	-1494.32
Butan-1-ol	-2156.59	-1887.01	-1878.63	-1974.08

Graph showing the heat of combustion of four alcohols

