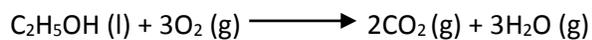


Calculating Enthalpy of Combustion for the First Five Alcohols

Background Information:

The heat produced when one mole of a substance is burned in excess oxygen is called the enthalpy of combustion. Methanol, ethanol, propanol, butanol and pentanol all belong to one homologous series; alcohols, with the functional group –OH. They have hydrogen bonds (specific kind of permanent dipole-dipole forces) and van der Waals' forces which increase as the length of the carbon chain increases. Complete combustion of alcohols produces carbon dioxide and water. An example of the reaction for enthalpy of combustion is given below:



For this reaction, the IB data booklet value (standard enthalpy change of combustion) is $-1367 \text{ kJ mol}^{-1}$ which shows that this reaction is exothermic.

Research Question:

What effect does the length of the carbon chain have on the enthalpy of combustion in primary alcohols?

Hypothesis:

The longer the carbon chain is in an alcohol, the greater its enthalpy of combustion is going to be.

Variables:

Independent Variable: Length of the carbon chain of the alcohol.	Dependent Variable: Mass of the alcohol burned.
Controlled Variables:	
<ol style="list-style-type: none">1. The temperature increase in water2. The mass of the water in the calorimeter3. Apparatus used4. The temperature and pressure of surroundings5. The distance between the calorimeter and the burner	

Method of control:

The independent variable is manipulated by changing the fuel in the burner each time to a different alcohol. For the controlled variables, temperature increase in water is set to be 30°C , after which the burner is to be removed to measure the change in mass on a balance. The mass of water is always 100 grams in the calorimeter. The same calorimeter, thermometer, balance and shape and type of burner

are used each time. The temperature of the surroundings is maintained via air conditioning in the lab. The distance between calorimeter and burner is measured by a ruler.

Apparatus:

Balance (± 0.01 g)

Thermometer (± 0.1 °C)

Aluminum calorimeter

Burners (Spirit lamps)

Wind shields

Clamps and stands

Materials:

Methanol, ethanol, propanol, butanol and pentanol in the spirit lamps

Match sticks

Distilled water

Wipes

Net Uncertainties (accounting for initial and final measurements if applicable)

Balance (for fuel)	± 0.02 g
Balance (for water)	± 0.01 g
Thermometer	± 0.2 °C

Procedure:

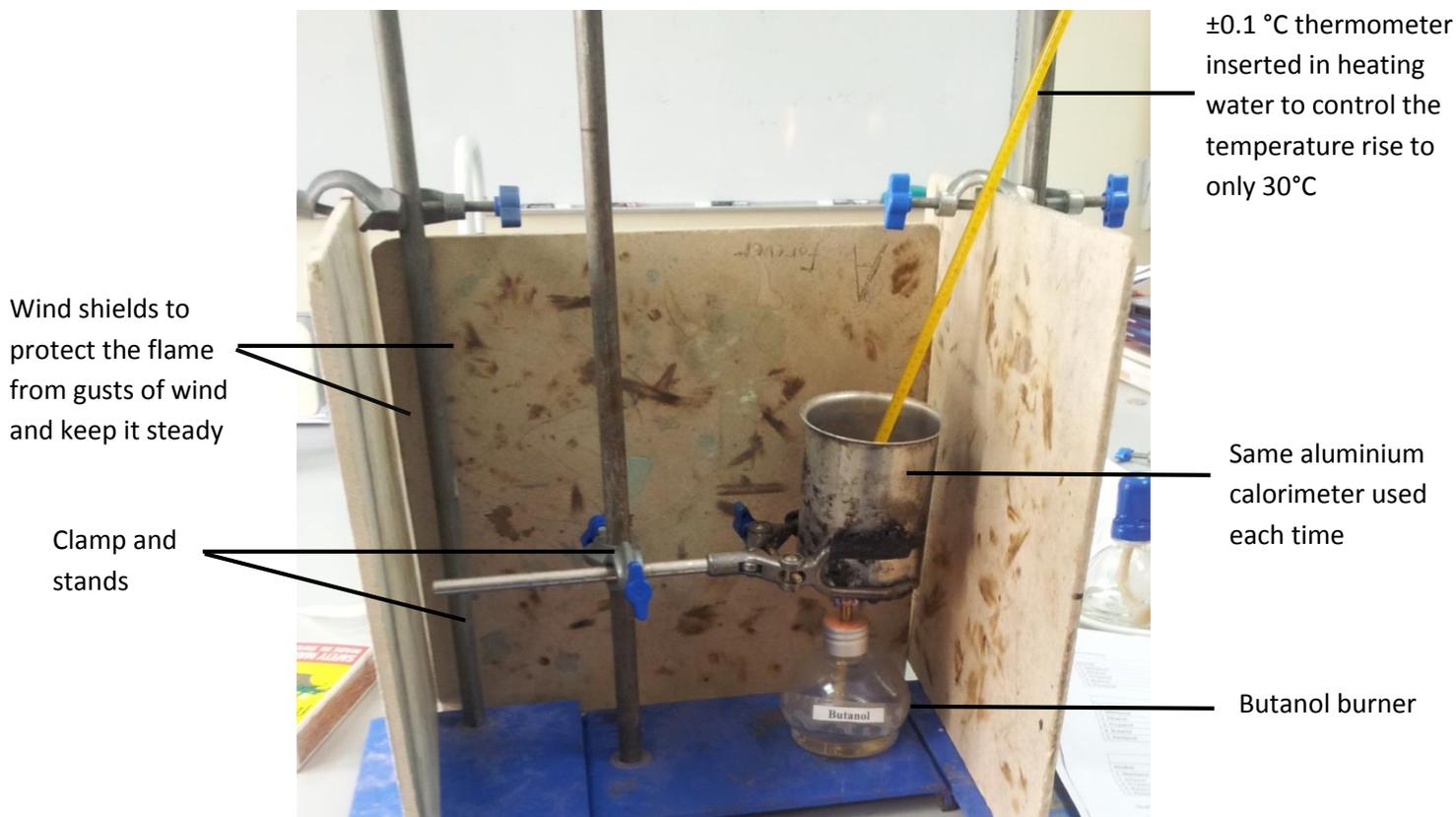
1. Measure a 100g of water and put it in the calorimeter clamped to a stand.
2. Fix wind shields on the clamps with the stands and place them so that the calorimeter is shielded from three sides.
3. Measure the initial mass of fuel, starting from methanol in the spirit burner. It's important to note that the lid should be closed; otherwise some of the fuel will vaporize and escape. Write down the initial mass.
4. Place a thermometer in the water and note down the initial temperature

5. Open the lid of the burner and light it. Immediately after that, place it under the calorimeter with water.
6. Stir the water frequently using the thermometer while it's being heated. This is to ensure that heat is transferred to the water as evenly as possible.
7. The thermometer is inserted the whole time. Keep reading the thermometer until there is an increase of 30°C, and note down any qualitative changes during that time.
8. Once there has been a temperature increase of 30°C, remove the burner, place the lid back on and measure its mass again. This has to be done swiftly, in order to minimize the amount of fuel escaping the burner.
9. Write down the final mass of the burner, and repeat steps 1 to 8 with all of the other 4 alcohols.
10. Repeat this whole experiment with all 5 alcohols at least two more times so there are three trials over all.

Risk Assessment:

Alcohols are not corrosive or harmful to the skin but they must not be ingested. For safety, wear goggles and a lab coat throughout. Use a pair of tongs to handle the hot calorimeter when adding or removing water again. Inform the teacher or a lab assistant immediately in case of a fire or a burn.

Photographs of the setup & apparatus:





±0.01 precision Digital balance used all times

Yellow flame; same distance between flame and calorimeter was maintained

Droplets of fuel formed on inner surface of the burner



Data Collection:

Masses of the alcohols before and after being used as a fuel to heat 100g water by 30°C

Alcohol	Trial 1		Trial 2		Trial 3	
	Initial mass/g ±0.01	Final mass/g ±0.01	Initial mass/g ±0.01	Final mass/g ±0.01	Initial mass/g ±0.01	Final mass/g ±0.01
1. Methanol	154.01	152.73	152.21	150.95	150.07	148.93
2. Ethanol	152.14	150.87	151.29	150.22	149.10	147.94
3. Propanol	181.41	180.64	180.54	179.78	179.72	178.92
4. Butanol	173.64	172.84	172.80	172.08	171.95	171.25
5. Pentanol	169.25	168.74	168.69	168.00	167.90	167.25

Table 1: Raw Data Table

Qualitative analysis:

- The flame for each of these fuels and trials was always yellow at the top.
- Black soot formed at the base of calorimeter at all times, but it got noticeably thicker and darker the higher the carbon chain of the alcohol was used.
- The burners themselves got warmer while they were heating up water. In some cases condensation droplets were visible on the inner surfaces as seen a photograph above.

- Although time wasn't a controlled variable in this experiment, the amount of time it took to raise the water by 30°C increased each time the carbon chain length was increased. This was perceptible even without the use of a timer.

Data processing:

The data above needs to be processed in order to draw meaningful results out of it. First of all, change of mass needs to be calculated. Since there were three trials in this experiment, it's best to take a mean of the mass change.

In this experiment, it is assumed that the heat change of the reaction is equal to the heat change of water i.e. all the energy lost by the fuel while it's burning is transferred to the water. Under this assumption, the following is an expression that can be used:

Heat change of reaction = heat change of water

$$= m_{H_2O} \times c_{H_2O} \times \Delta T_{H_2O}$$

Where m is the mass of water, c is the specific heat capacity of water and ΔT is the temperature change of water. Enthalpy of combustion is measured in kJmol^{-1} therefore this value is divided by the number of moles of the fuel and 1000. The sample calculation for methanol for all of the above is done here.

Change in mass: $154.01 - 152.73 = 1.28 \text{ g}$, $152.21 - 150.95 = 1.26 \text{ g}$, $150.07 - 148.93 = 1.14 \text{ g}$

Mean change in mass = 1.23 g

Number of moles of methanol = mass/molar mass = $1.23 / (12.01 + 3.03 + 17.01) = 0.04 \text{ mol}$

Heat change in water = $m \times c \times \Delta T = 100 \times 4.18 \times 50 = 20900 \text{ Joules}$

Heat change of the reaction = $20900 / 0.04 = -546069.29 \text{ Jmol}^{-1} = -546.07 \text{ kJmol}^{-1}$

(A negative sign is added at the end because combustion is always an exothermic reaction)

Alcohol	Trial	Change in mass/ g ±0.02	Mean change in mass/ g ±0.02	No. of moles of alcohol	Heat change of water/ J	Enthalpy of combustion/ Jmol ⁻¹	Enthalpy of combustion/ kJmol ⁻¹
1. Methanol	1	1.28	1.23	0.04	20900.00	-546069.29	-546.07
	2	1.26					
	3	1.14					
2. Ethanol	1	1.27	1.17	0.03	20900.00	-825490.29	-825.49
	2	1.07					
	3	1.16					
3. Propanol	1	0.77	0.78	0.01	20900.00	-1617552.36	-1617.55
	2	0.76					
	3	0.80					
4. Butanol	1	0.80	0.74	0.01	20900.00	-2093954.05	-2093.95
	2	0.72					
	3	0.70					
5. Pentanol	1	0.51	0.62	0.01	20900.00	-2988248.11	-2988.25
	2	0.69					
	3	0.65					

Table 2: Processed data table

Total percentage uncertainty:

$$\text{Percentage uncertainty} = \left(\frac{\text{net uncertainty}}{\text{measured value}} \right) \times 100\%$$

The net uncertainties for mass of water, temperature and mass of fuel were mentioned above, and can be summarized in the following expression respectively for 100g water and 30°C temperature rise. The mass of fuel varies so it's given the variable x . The total percentage uncertainties for each fuel is calculated overleaf.

$$\begin{aligned} & \frac{0.01}{100} \times 100 + \frac{0.2}{30} \times 100 + \frac{0.02}{x} \times 100 \\ & = \pm \left(0.68 + \frac{2}{x} \right) \% \end{aligned}$$

	Mean mass of the fuel used/g ± 0.02	Percentage uncertainty of fuel used	Total percentage uncertainty
1. Methanol	1.23	$\pm 1.63 \%$	$\pm 2.31 \%$
2. Ethanol	1.17	$\pm 1.71 \%$	$\pm 2.39 \%$
3. Propanol	0.78	$\pm 2.58 \%$	$\pm 3.26 \%$
4. Butanol	0.74	$\pm 2.70 \%$	$\pm 3.38 \%$
5. Pentanol	0.62	$\pm 3.24 \%$	$\pm 3.92 \%$

Table 3: Calculations of total percentage uncertainty

Absolute uncertainty:

Absolute uncertainty can be calculated by multiplying the total percentage uncertainty to the enthalpy of combustion of the fuel in kJ mol^{-1} .

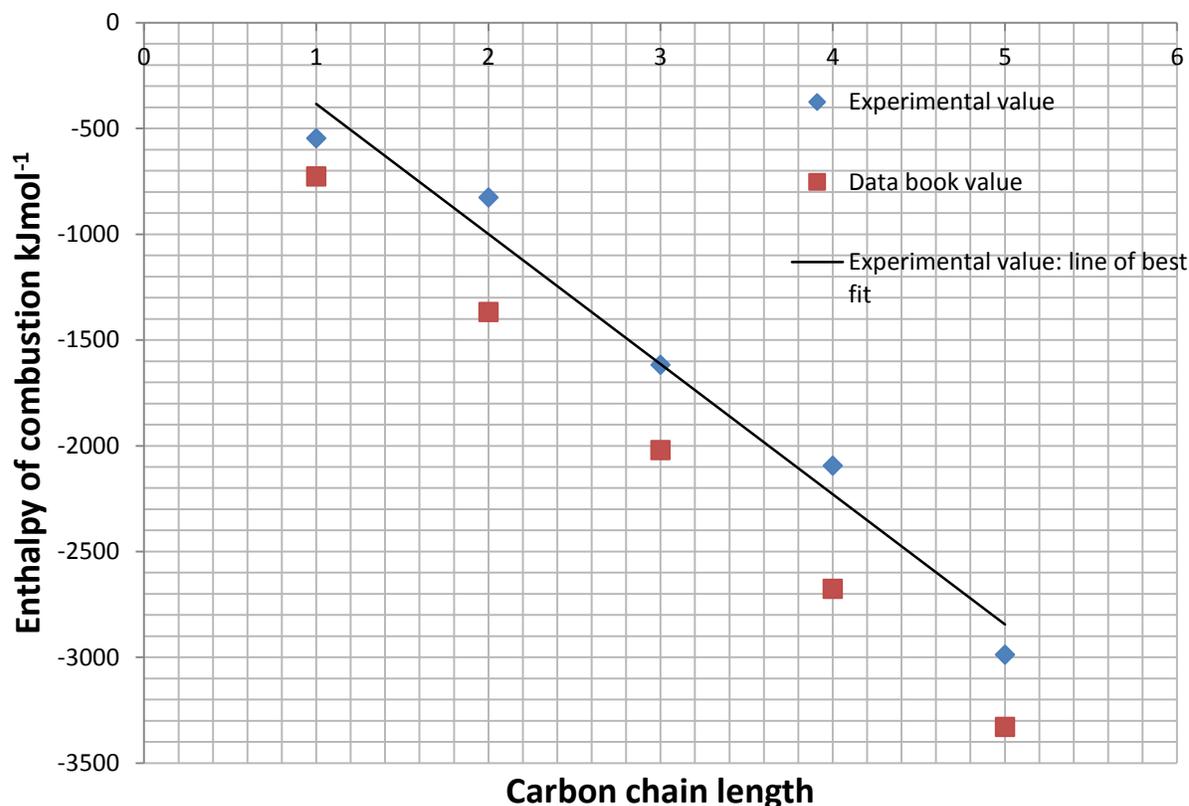
In the case of methanol,

$-\frac{2.31}{100} \times -546.07 = -12.6142 \text{ kJ mol}^{-1}$ is the maximum amount of methanol that can be more or less than the value written in table 2 ($-546.07 \text{ kJ mol}^{-1}$)

	Absolute uncertainty / kJ mol^{-1}
1. Methanol	-12.61
2. Ethanol	-19.73
3. Propanol	-52.73
4. Butanol	-70.78
5. Pentanol	-117.14

With all of the data processed above, a line graph can be produced to show the relationship and trend between the increasing carbon chain length in an alcohol and its enthalpy of combustion, both in terms of this experiment's values and data book values.

The enthalpy of combustion of methanol, ethanol, propanol, butanol and pentanol



Conclusion:

The enthalpy of combustion of an alcohol increases as the carbon chain length increases. The graph produced a downward sloping line because enthalpy of combustion values are negative; the higher the negative value, the greater the enthalpy of combustion. This conclusion is in agreement with the hypothesis and the trend given above, except that the experimental results didn't show a linear increase in enthalpy of combustion.

The final values of enthalpy of combustion in ascending order of carbon chain are $-546.07 \text{ kJmol}^{-1}$, $-825.49 \text{ kJmol}^{-1}$, $-1617.55 \text{ kJmol}^{-1}$, $-2093.95 \text{ kJmol}^{-1}$ and $-2988.25 \text{ kJmol}^{-1}$. The differences in these values again describe that the increase is not linear, i.e. close to equal between the alcohols. Percentages of total uncertainty were different for each alcohol as well. The bigger the carbon chain length was, the greater uncertainty was produced, ranging from $\pm 2.31\%$ for methanol to $\pm 3.92\%$ for pentanol. This is because mean change in mass before and after using pentanol for heating water was only 0.62 g whereas the mean change in mass of methanol was nearly double that amount; at 1.23 g.

The principal reason for these observations is that increasing the carbon chain length increases the size of the molecule significantly. The molecular formula of methanol is CH_3OH , ethanol is $\text{C}_2\text{H}_5\text{OH}$, and propanol is $\text{C}_3\text{H}_7\text{OH}$ and so on. Increase in one carbon atom results in two more hydrogen atoms and over all 3 more sigma bonds on the carbon atoms. The molar mass of methanol is 32 g mol^{-1} and there's an increase of 14g each time a carbon atom (and consequently two hydrogen atoms) are added. Increase in molecular mass greatly affects van der Waal's forces (temporary and weak intermolecular forces). It's harder to break bigger carbon chain molecules because it takes longer to break these intermolecular bonds. This was observed in the qualitative data above, methanol raised the temperature of water fairly quickly, but pentanol took a lot of time. Apart from van der Waal's forces, all alcohols also contain hydrogen bonds which are the strongest intermolecular force, but these are present equally in all primary alcohols.

The experimental values produced as a result of this investigation can be compared to standard enthalpy of combustion values. The dotted red line on the graph on the previous page represents standard values taken from the IB data booklet; these are higher than the experimental values. The percentage error is a measure of how close the experimental value is to the data book value.

$$\text{Percentage error} = \left(\frac{\text{data book value} - \text{experimental value}}{\text{data book value}} \right) \times 100$$

	Data book value/ kJmol^{-1}	Experimental value/ kJmol^{-1}	Percentage error
1. Methanol	-726	-546.07	24.78 %
2. Ethanol	-1367	-825.49	39.61 %
3. Propanol	-2021	-1617.55	19.96 %
4. Butanol	-2676	-2093.95	21.75 %
5. Pentanol	-3329	-2988.25	10.24 %

Table 4: Percentage error calculations

Evaluation:

The large percentage error calculated in the previous page indicates that this experiment has some flaws. The set up itself was well designed for gathering data, and it was simple to replicate. The number of trials should be a minimum of 5 to make any proper judgment, and this wasn't possible due to time constraints. The main flaw of this experiment, however, is its core assumption that all the heat produced by the combustion is transferred to the water when in fact there are many heat losses to the surroundings.

Heat losses form the majority of the percentage error. There's no insulation on the calorimeter and no insulating card covering the calorimeter and retaining the heat inside. As a result, a lot of the heat escapes from the water and is lost to the surroundings. Some of the heat is also absorbed by the calorimeter itself. The experiment doesn't take this into account and doesn't involve calculations of heat gained by aluminium when that could have been calculated (using $m \times c \times \Delta T$ equation) and

subtracted from the heat produced by fuel as a more accurate representation of the heat transferred to water.

One of the other for this large percentage error is the incomplete combustion of the fuel that was noted above in the qualitative analysis (yellow flame and formation of soot). This was because the fuel didn't receive enough oxygen to burn completely and indicates that the fuel was used inefficiently because incomplete combustion releases less energy compared to complete combustion.

The uncertainties of the equipment were not too large as noted above in table three. The uncertainty increased as the carbon chain length increased but it still has far less an effect on the outcome of the experiment when compared to heat losses to the environment.

It's significant that the percentage error for the alcohols isn't similar to each other (largest percentage error was ethanol at 39.61% and the smallest was methanol at just 10.24%). This indicates that the conditions of the surroundings, specifically the temperature, weren't controlled effectively. Although an air conditioner was used throughout the experiment at a constant temperature, it wasn't enough as the lab door would open sometimes and the heat and sunlight outside changed frequently.

There's also a possibility of random errors in this experiment, and errors that took place due to reaction time in looking out for temperature rise, closing the lid of the fuel as soon as it reaches 30°C and weighing it immediately. These errors, however, are much harder to evaluate properly and control.

Improvements:

Improvement	How it enhances the investigation
1. Using insulation such as air foam around the calorimeter	Minimizes one of the sources of heat loss
2. Insulating card to cover the water	Retains the energy inside the heating water rather than letting it escape to the surroundings
3. Use of a copper calorimeter and calculations regarding heat absorbed by calorimeter itself	Copper is a better conductor of heat compared to aluminum. If heat energy gained by copper is calculated, it can be subtracted from the heat of combustion of the fuel to provide a more accurate calculation of the heat transferred to water.
4. Burn the fuel in excess oxygen	This will stop incomplete combustion and soot formation and release more energy once the fuel is undergoing through complete combustion only.
5. Use of an electric thermometer	This will reduce the uncertainties a great deal and therefore make the experiment more precise.