

## Comparing The Enthalpy Change Of Combustion Of Different Alcohols

The aim of my experiment is to investigate the enthalpy of combustion of a range of alcohols. The standard enthalpy of combustion is the enthalpy change that occurs when 1 mole of a fuel is burned completely in oxygen under standard conditions – 1 atmosphere pressure and 298K. All combustion reactions are exothermic which is why I am expecting all the values for the enthalpy change of combustion to always be negative.

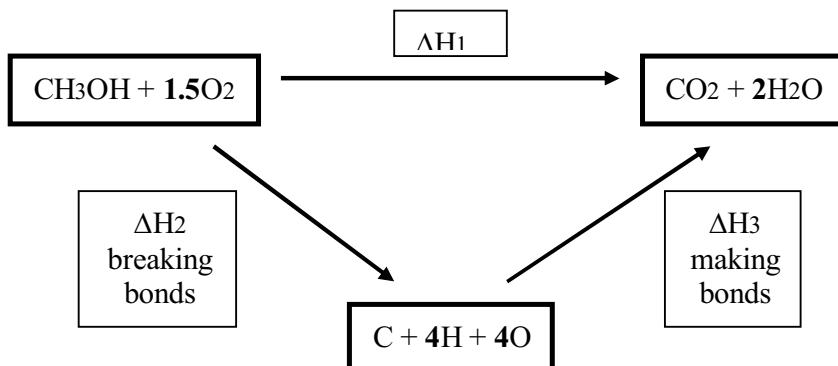
### Prediction

I predict that the greater the number of carbon atoms there are in the alcohol molecule, the greater the enthalpy change of combustion it will have. This is because in a chemical reaction energy is needed in order to break bonds and energy is released when bonds are made. If I were to look at these two values; the energy required to break the bonds of the reactants and the energy released when the bonds of the product are made then I am able to work out the enthalpy change of combustion of the alcohol. In order to do this we need to know the bond enthalpies of the bonds in the process. The quantity of energy needed to break a particular bond in a molecule is called the bond enthalpy. Below is a table containing the bond enthalpies of the bonds that occur in the combustion of an alcohol.

Bonds	Average bond enthalpy/kJ mol <sup>-1</sup>
C-C	+347
C-H	+413
C-O	+358
O-H	+464
O=O	+498
C=O	+805

We use the average bond enthalpies as the exact value of a bond enthalpy depends on the particular compound in which the bond is found.

By looking at the equation for the reaction that occurs when an alcohol burns, we realise that the reaction involves both breaking bonds and making new ones. From the equation of the process we can tell how many of the different number of bonds are broken and made and so work out the enthalpy change of combustion. We can work out the enthalpy of combustion of methanol by using the bond enthalpy values:



We can use the enthalpy cycle above to work out the value for the enthalpy change of combustion of methanol, represented by  $\Delta H_1$ . The calculation is done as shown below:

$\Delta H_2$  = enthalpy change when bonds are broken

$$= 3 \times E(\text{C-H}) + 1 \times E(\text{C-O}) + 1 \times E(\text{O-H}) + 1.5 \times E(\text{O=O})$$

$$= 3(413) + 358 + 464 + 1.5(498)$$

$$= 2808 \text{ kJ mol}^{-1}$$

$\Delta H_3$  = enthalpy change when bonds are made

$$= -[2 \times E(\text{C=O}) + 4 \times E(\text{O-H})] \quad (\text{the minus sign occurs because energy is released when the bonds are made.})$$

$$= -[2(805) + 4(464)]$$

$$= -3466 \text{ kJ mol}^{-1}$$

So the enthalpy change of combustion,  $\Delta H_1$ , is given by:

$$\Delta H_1 = \Delta H_2 + \Delta H_3 = +2808 \text{ kJ mol}^{-1} + (-3466 \text{ kJ mol}^{-1})$$

$$= -658 \text{ kJ mol}^{-1}$$

The balanced equations for the combustion of the five alcohols I am going to be using are:

Methanol  $\text{CH}_3\text{OH(l)} + 1.5\text{O}_2(\text{g}) \rightarrow \text{CO}_2(\text{g}) + 2\text{H}_2\text{O(l)}$

Ethanol  $\text{C}_2\text{H}_5\text{OH(l)} + 3\text{O}_2(\text{g}) \rightarrow 2\text{CO}_2(\text{g}) + 3\text{H}_2\text{O(l)}$

Propanol  $\text{C}_3\text{H}_7\text{OH(l)} + 4.5\text{O}_2(\text{g}) \rightarrow 3\text{CO}_2(\text{g}) + 4\text{H}_2\text{O(l)}$

Butanol  $\text{C}_4\text{H}_9\text{OH(l)} + 6\text{O}_2(\text{g}) \rightarrow 4\text{CO}_2(\text{g}) + 5\text{H}_2\text{O(l)}$

Pentanol  $\text{C}_5\text{H}_{11}\text{OH(l)} + 7.5\text{O}_2(\text{g}) \rightarrow 5\text{CO}_2(\text{g}) + 6\text{H}_2\text{O(l)}$

Below is a prediction table for the predicted enthalpy of combustion values for the other alcohols worked out in the same way as the one above:

Alcohol	Enthalpy change when bonds are broken (kJ mol <sup>-1</sup> )	Enthalpy change when bonds are made (kJ mol <sup>-1</sup> )	Enthalpy of combustion (kJ mol <sup>-1</sup> )
Methanol <chem>CH3OH</chem>	2808	-3466	-658
Ethanol <chem>CH3CH2OH</chem>	4728	-6004	-1276
Propan-1-ol <chem>CH3CH2CH2OH</chem>	6648	-8542	-1894
Butan-1-ol <chem>CH3CH2CH2CH2OH</chem>	8568	-11080	-2512
Pentanol <chem>CH3CH2CH2CH2CH2OH</chem>	10488	-13618	-3130

From the table above we can see that as the alcohol becomes larger, energy required when bonds are broken and the energy released as bonds are made both increased which is what I would expect. The enthalpies of combustion of the alcohols would also increase. We can see that this figure increases constantly, by  $-618 \text{ kJ mol}^{-1}$  as  $\text{CH}_2$  is added. The reason for the equal increase in the change in enthalpy of combustion is because a  $\text{CH}_2$  group is

added to the alcohol chain each time it gets larger so we would expect to get the same energy out each time. This is what I expect will happen when I carry out my experiment.

In order to make my experiment more accurate, I am going to repeat each alcohol twice as I expect this to be a sufficient amount as the random errors are going to be fairly small.

### **Risk Assessment**

There are many factors to consider when carrying out this experiment. A vital part is to carry it out in safety. So I am going to follow a set of guidelines in order to do the experiment in safety.

1. The alcohols are extremely flammable liquids. I should keep bottles stoppered when not in use and well away from naked flames.
2. I will avoid skin contact and will not breathe in vapours as they can be harmful and toxic.
3. I will not open the spirit burner (to refill) in the laboratory with naked flames.
4. The apparatus will be hot during and after the experiment and so care should be taken when handling it and I should wait until the equipment has cooled down sufficiently before moving it

### **Preliminary work**

Method

1. Put cold water in a copper container then weigh them and record the water temperature.
2. Secure fibre glass around the container to reduce energy loss and place the container between the triangle of a tripod so it is supported over a spirit burner.
3. Weigh the spirit burner.
4. Replace the spirit burner under the container and light the wick.
5. Go on heating until the temperature has risen by about 50 -60 degrees.
6. Extinguish the burner and note the highest temperature reached.
7. Weigh the burner to see what mass of fuel has been burned.

### **Changes Made To My Initial Method And Why**

To reduce errors in my final method I will make the following changes to my initial method:

1. I am now going to place the copper container into a tin can for insulation. But I need to take into consideration that heat energy will also be

transferred to the tin can as well as the copper container from the flame, so I will include their total mass in my calculations.

2. I am now not going to use fibre glass for insulation as it cannot be placed over the sides of the tin can. Instead I am going to use a draught shield which will reduce the amount of energy lost to the surroundings. The draught shield will have holes in the side to allow oxygen to the flame and carbon dioxide to leave.
3. A cork lid is placed on the can to reduce energy loss through the top of the container and holes for a thermometer and a stirrer are made. A stirrer will be used to maintain a constant water temperature throughout the container.
4. Fresh cold water will be used for each experiment in order to keep the start temperature of the water similar and this would also mean that I would have the same system each time.
5. The burner will be removed from under the copper container before the water reaches the target end water temperature of 80-90 degrees Celsius. This is because there is a temperature lag on the thermometer.
6. The water will be heated until the temperature has risen to about 80-90 degrees Celsius. As the temperature will be measured to a higher amount this will mean that the results will be more accurate as the temperature range is greater.
7. Once the burner is removed after the experiment is over, it will still be hot from the experiment and so the alcohol may still be evaporating from the open spirit burner. So I will extinguish the burner flame by placing the burner lid over the lit wick, which will keep the alcohol from evaporating out of the burner.
8. I am going to do three repeat experiments for all five alcohols (methanol, ethanol, propan-1-ol, butan-1-ol and pentanol) in order to gain more precise results for calculating the enthalpy change of combustion. As the more repeats that are carried out, the more accurate the results are.
9. I am going to use 5 different alcohols. These are: methanol, ethanol, propan-1-ol, butan-1-ol and pentanol. I will use propan-1-ol and butan-1-ol as they both have very similar structural arrangements compared with methanol, ethanol and pentanol. All alcohols that I will use have a consistent increase in carbon atoms and also have an OH group joined onto the end of the carbon atom and are all straight chain alcohols. I will not use isomers of the alcohols. As these alcohols are very similar, the main difference (varying factor) being an increase in chain length due to an increase in carbon atoms, the choice of alcohols will enable me to compare the change in enthalpy of combustion between them.

In order to calculate the enthalpy change of combustion of the alcohols, I will do the following:

- a) Measure the mass of the burner at the start of the experiment (before it has been lit) and after the experiment (once the flame has been put out). I will then calculate the change in mass of the spirit burner from the beginning and end of the experiment. The volume of water does not need to be measured because I have measured its mass.
- b) I will use mass of water between 80grams and 120grams in order to make the repeat results as similar and therefore reliable as possible.

- c) The temperature of the water in the copper container will be measured before the experiment has begun and at the end of the experiment using a thermometer. I will then calculate the change in temperature of the water before and after the experiment.
- d) I will use 5 different alcohols, which is a sensible range in order to gather sufficient data to find a relationship between the enthalpy change of combustion and the number of carbon atoms in the alcohol.
- e) wait for the temperature to stay 5 alcohol which will give me a good range and so my results being more reliable

## Results

Alcohol	Temperature of water at start	Temperature of water at end	Temperature Change of water	Mass of water (g)	Mass of copper container and aluminium can (g)	Total mass (g)	Start mass of burner (g)	End mass of burner (g)	Mass of fuel used
methanol	19	84	65	96.98	68.20	165.18	142.48	137.94	4.54
	23	80	57	102.44	68.20	170.64	142.90	139.08	3.82
Ethanol	24	84	60	88.29	68.20	156.49	159.08	156.32	2.76
	18	87	69	102.16	68.20	170.36	153.53	150.20	3.33
propan-1-ol	21	83	62	103.47	68.20	171.67	141.85	139.97	1.88
	15	79	64	109.5	68.20	177.70	170.39	167.55	2.84
butan-1-ol	18	84	66	94.45	68.20	162.65	135.35	132.47	2.88
	16	92	76	90.76	68.20	158.96	170.69	167.50	3.19
Pentanol	27	86	59	103.17	68.20	171.37	143.41	140.90	2.51
	24	82	58	100.58	68.20	168.78	138.15	135.71	2.44

I have chosen to repeat the experiments for each alcohol twice. Also I have taken results over a large temperature range. This means that all the values in my results will be greater and as values increase so does their accuracy and therefore I am expecting more reliable results.

To work out the enthalpy change of combustion for the alcohols, I need to first work out the energy transferred to both the copper container and the water. I

do this by using two constants ; the specific heating capacity of water and copper. I also use the temperature rise of the water. So I use the relationship:

$$\text{Energy transferred} = m_1 c_1 \Delta T + m_2 c_2 \Delta T$$

Where  $c_1$  is the heating capacity of water ( $4.17 \text{ Jg}^{-1} \text{K}^{-1}$ ) and  $c_2$  is the heating capacity of copper ( $0.387 \text{ Jg}^{-1} \text{K}^{-1}$ ).

And  $m_1$  is the mass of water and  $m_2$  is the mass of the copper container.

And  $\Delta T$  is the temperature change. Below I have worked out the energy transferred to the water and copper container when methanol was burned in our first experiment from the table of results:

$$\begin{aligned} \text{Energy transferred} &= (165.18 \text{ g} \times 4.17 \text{ Jg}^{-1} \text{K}^{-1} \times 65^\circ \text{C}) + (68.20 \text{ g} \times 0.387 \text{ Jg}^{-1} \text{K}^{-1} \times 65^\circ \text{C}) \\ &= 46487.61 \text{ J} \end{aligned}$$

This is the total energy transferred to the water and copper container during the combustion of the alcohol and we now need to change this value to energy transferred per mole of alcohol burned in order to find out how much energy per mole is released by the alcohol. To do this I use the formula:

$$\begin{aligned} \Delta H_c &= (\text{Energy transferred} / \text{Mass of fuel burned}) \times \text{Relative molecular mass of fuel} \\ &= (46487.61 \text{ J} / 4.54 \text{ g}) \times 32 \\ &= 327665.9736 \\ &= 328 \text{ KJ mol}^{-1} \text{ for Methanol} \end{aligned}$$

Below is a table to show the enthalpy change of combustion of the alcohols from my results.

Alcohol	Experiment	Energy transferred/Mass of fuel burned (J/g)	RMM of fuel	Enthalpy change of combustion of fuel (KJmol <sup>-1</sup> )	Change in enthalpy of combustion as carbon atoms increase (KJmol <sup>-1</sup> ) taken from the graph.
Methanol	1	46487.61/4.54	32	-328	320
	2	42063.8454/3.82	32	-352	
Ethanol	1	40737.402/2.76	46	-679	320
	2	50838.8274/3.33	46	-707	
Propan-1-ol	1	46019.9526/1.88	60	-1469	320
	2	49113.7536/2.84	60	-1038	
Butan-1-ol	1	46506.4974/2.88	74	-1195	320
	2	52383.5016/3.19	74	-1215	
Pentanol	1	43719.3717/2.51	88	-1533	320
	2	42351.948/2.44	88	-1527	

The enthalpy change of combustion values are negative because the reaction was an exothermic reaction.

My prediction that “as the number of carbon molecules increases, so would the enthalpy change of combustion”, has been proved correct as shown in the

table and on the graph. However the values calculated from my experiments shows that less energy has been transferred to the copper can and water compared with my theoretical values. This is mainly due to a large proportion of heat energy from the flame being transferred to the surroundings. Energy would be transferred to the surrounding air particles which may have lead to a smaller increase in temperature and in turn the value for the enthalpy change of combustion was lower. Also another factor that may have contributed to the lower values could have been a large amount of energy loss from the evaporation of water due to the experiments being heated to approximately 85 degrees Celsius each time.

The figure for the enthalpy change of combustion was negative because the reaction was endothermic. This is also proved by my results as they are negative. My results show that as the number of carbon atoms increase, more energy is released as a number of stronger bonds are made. As a carbon bond breaks it requires  $347\text{kJmol}^{-1}$  of bond enthalpy to break and once broken the carbon atom bonds with an oxygen molecule which gives out more than twice the amount of energy needed to break the carbon bond. So the amount of energy per mol transferred to the water and copper container has increased as the number of carbon atoms increases.

I can say that my average straight line for the results is reliable because the error bars on the graph are so small. From the graph we can see that there is a constant increase in the change of enthalpy of combustion of the alcohols as the number of carbon atoms increase. This increase is  $-320\text{kJmol}^{-1}$  which is almost exactly half the predicted value which was  $-618\text{kJmol}^{-1}$ . Thus I can say that reactions were about 50% efficient. I can work out the accuracy of my results by comparing the average enthalpy change of combustion of an alcohol by my predicted value. The efficiency is calculated and is shown below:

Alcohol	Average practical enthalpy of combustion/Predicted enthalpy of combustion	Accuracy of results (%)
Methanol	-300/-618	49
Ethanol	-620/-1276	49
Propan-1-ol	-940/-1894	50
Butan-1-ol	-1260/-2512	50
Pentanol	-1580/-3130	50

The table shows that all my experiments were about 50% accurate which means that the energy transfer from the flame to the water and copper container was very inefficient (about 50%).

I have found an anomalous result for the enthalpy of combustion in my first experiment for propan-1-ol. The graph shows that the value is a lot higher than my second experiment and also it does not follow the trend of the other values being close to the line of best fit. The reason for the anomaly could have been because there may not have been standard condition during the experiment or from the results shown we can see that less fuel was burned to

raise the temperature level of water, so the experiment could have been more efficient than the others.

### **Evaluation**

The greatest error in the experiments was heat loss (energy transferred to the atmosphere and equipment). Improvements I could make to my experiment to make it more accurate would be to use a draft excluder as well as insulation using glass wool. These changes would reduce energy loss to the surroundings; to equipment and the air particles so increasing the amount of energy transferred and making the experiment more efficient. Incomplete combustion also forms part of the error as not all of the fuel was being burnt and so we would need to take into account the amount of carbon monoxide produced and so also calculate the energy released when it is produced.

I used different burners for each experiment, which would have led to errors because the alcohols would have burned differently each time. For example, the burners have different wicks that burn differently, some better than others so more alcohol may have been burned. I should have used a new wick of the same type for each experiment in order for the alcohols to be soaked into the wick equally.

From the experiments I have done, there were two types of errors which affected the outcome of my results. These were random and systematic errors.

In my experiment I encountered errors due to the accuracy of the measurements. This is a random error. Below I have drawn a table to show the total error due to the measurements I took.

	Quantity measured	% error calculation	% error	Total % error
Mass of water+copper container	165.18g	$2 \times (0.005/165.18) \times 100$	0.006	3.09
Mass of fuel using balance	142.48g	$2 \times (0.005/142.48) \times 100$	0.007	
Temperature change using thermometer	65	$2 \times (1/65) \times 100$	3.077	

From the table we can see that the percentage error for the mass of water and copper container and the mass of fuel was very small, less than 1%, which tells us that the error is so small that it would not affect the final value of the change in enthalpy of combustion.

But we can see that there was a significantly higher percentage error in the temperature change. This error could have been reduced by using a digital thermometer which reads to 2 decimal places. This error would increase the enthalpy change of combustion by a small margin which is not a



large amount in comparison to the whole figure and also would not change my line of best fit for my practical results. I can show this by incorporating this 3.077% error in temperature change in my calculation for the enthalpy change of combustion of methanol. The original formula:

$$\begin{aligned}\text{Energy transferred} &= (165.18\text{g} \times 4.17\text{Jg}^{-1}\text{K}^{-1} \times 65^\circ\text{C}) + (68.20\text{g} \times 0.387\text{Jg}^{-1}\text{K}^{-1} \times 65^\circ\text{C}) \\ &= 46487.61\text{J}\end{aligned}$$

We can see that the temperature change is  $65^\circ\text{C}$ . The percentage error for temperature change is 3.077%. I multiply this increase by the original value:

$$65^\circ\text{C} \times 1.03077 = 67^\circ\text{C}$$

We can substitute  $67^\circ\text{C}$  in place of  $65^\circ\text{C}$  in our original formula:

$$\begin{aligned}\text{Energy transferred} &= (165.18\text{g} \times 4.17\text{Jg}^{-1}\text{K}^{-1} \times 67^\circ\text{C}) + (68.20\text{g} \times 0.387\text{Jg}^{-1}\text{K}^{-1} \times 67^\circ\text{C}) \\ &= 47918.00\text{J}\end{aligned}$$

We can calculate the new enthalpy change of combustion of ethanol incorporating the error:

$$\begin{aligned}\Delta H_c &= (\text{Energy transferred} / \text{Mass of fuel burned}) \times \text{Relative molecular mass of fuel} \\ &= (47918.00\text{J} / 4.54\text{g}) \times 32 \\ &= 337748.00 \\ &= 338\text{kJ mol}^{-1} \text{ for Methanol}\end{aligned}$$

The new change in enthalpy of combustion of methanol will be  $328\text{kJ mol}^{-1} + 10\text{kJ mol}^{-1}$  or  $-10\text{kJ mol}^{-1}$ . We can see that the error will be small in comparison to the whole value and so I do not feel that this error is significant enough to incorporate into my graph.

Therefore the total error due to measurements was 3.09% which is not a significant amount to affect my results or my graph dramatically so I did not take into account these errors in my calculations. But I could have reduced the error due to temperature change using the thermometer by using a data logger as it is more accurate and also gives almost instant temperature readings.

There were also errors due to calculations of the change in enthalpy of combustion value. This error is shown below:

The change in enthalpy of combustion of ethanol ( $\text{CH}_3\text{CH}_2\text{OH}$ ) for my first experiment was  $-679\text{kJ mol}^{-1}$  which is 600 plus or minus 10 because the value is in its hundreds. So the percentage error for each of these values is 1.7%, not a significant amount to change my graph by a large amount.

Modifications of preliminary work justified:

I used a cork lid on the can which greatly reduced the amount of energy loss through the top of the container and also kept in some evaporating vapour inside the container. This meant that my measurements of temperature could be more reliable.

I used a tin foil draft excluder which reduced the draft from getting to the burner flame but I found that not enough oxygen was being supplied and so the flame went out a couple of times. To combat this problem I could have used an oxygen generator to supply to the flame. The tin foil resulted in my experiment to be less accurate because not enough oxygen was being supplied to the flame which in turn would have led to a lower enthalpy change of combustion value.

I used a tin can to insulate the copper container. This did not work and the heat energy from the flame was transferred to the water, then to the copper container and also then to the tin can. I included this in my calculations which reduced the accuracy of my final results because I had to perform two calculations instead of just one (if I had insulated the copper container with fibre glass, then placed this in the copper container then the heat energy would not have been transferred and there would have been no need for the extra calculation

### **Bibliography**

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