COMPARING THE ENTHALPY CHANGE OF COMBUSTION OF DIFFERENT ALCHOHOLS.

Aim

The aim of my experiment will be to find out which alcohols have a higher enthalpy change of combustion. The comparison of the enthalpy changes of these fuels will then determine the alcohol efficiency and effectiveness. I will experiment on the first 5 consecutive primary alcohols. These are; methanol, ethanol, propan-1-ol, butan-1-ol, pentan-1-ol and hexan-1-ol. The reason why I chose these fuels is because they are the most reliable and accurate fuels to compare within the group; which also have the smallest varia ble, 'add one carbon' each time, to the aliphatic chain. All combustion reactions are exothermic which is why I am expecting all the values for the enthalpy cha nge of combustion to always be negative.

$CH_3OH + 1.5O_2 \longrightarrow CO_2 + 2H_2O$ METHANE

$CH_3CH_2OH + 3O_2 \longrightarrow 2CO_2 + 3H_2O$ ETHANOL

$CH_3CH_2CH_2OH + 4.5O_2 \longrightarrow 3CO_2 + 4H_2O$ PROPAN-1-OL

$CH_3CH_2CH_2CH_2OH + 6O_2 \longrightarrow 4CO_2 + 5H_2O$ BUTAN-1-OL

$CH_3CH_2CH_2CH_2CH_2OH + 7.5O_2 \longrightarrow 5CO_2 + 6H_2O$ PENTAN-1-OL

$CH_3CH_2CH_2CH_2CH_2CH_2OH + 9O_2 \longrightarrow 6CO_2 + 7H_2O$ HEXAN-1-OL

Prediction

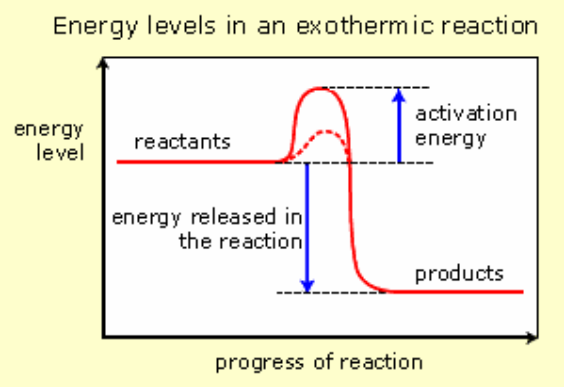
I believe that hexan-1-ol will have the highest enthalpy of combustion because there are more bonds to break and form and the energy released when bonds form is greater than energy ne eded to break bonds, this means that the reaction is exothermic and there is a higher temperature rise.

The molecular formulas are shown below. The general fo rmula for alcohols series are $C_nH_{2n+1}OH$.This means you move across the series the amount of carbon and hydrogen atoms increase. This also means that the relative atomic mass increases. Although more energy is needed to break up hexan-1-ol than that of methanol, the energy released when new bond form is greater due to its higher mass and higher length of aliphatic chain, therefore it's more exothermic. The stored energy of the reactants is higher than the stored energy of the reaction. The difference in energy is released to the surroundings when the fuel and oxygen react.

$CH_3OH + 1.5O_2 \longrightarrow CO_2 + 2H_2O$ METHANE

$CH_3CH_2CH_2CH_2CH_2CH_2OH + 9O_2 \longrightarrow 6CO_2 + 7H_2O$ HEXAN-1-OL

As seen above in methanol only 1 CO_2 and $2H_2O$ have been formed, which is a lot smaller than the new bonds formed in hexan-1-ol, $6CO_2$ and $7H_2O$ are formed and energy released from these are greater and make the reaction more exothermic.



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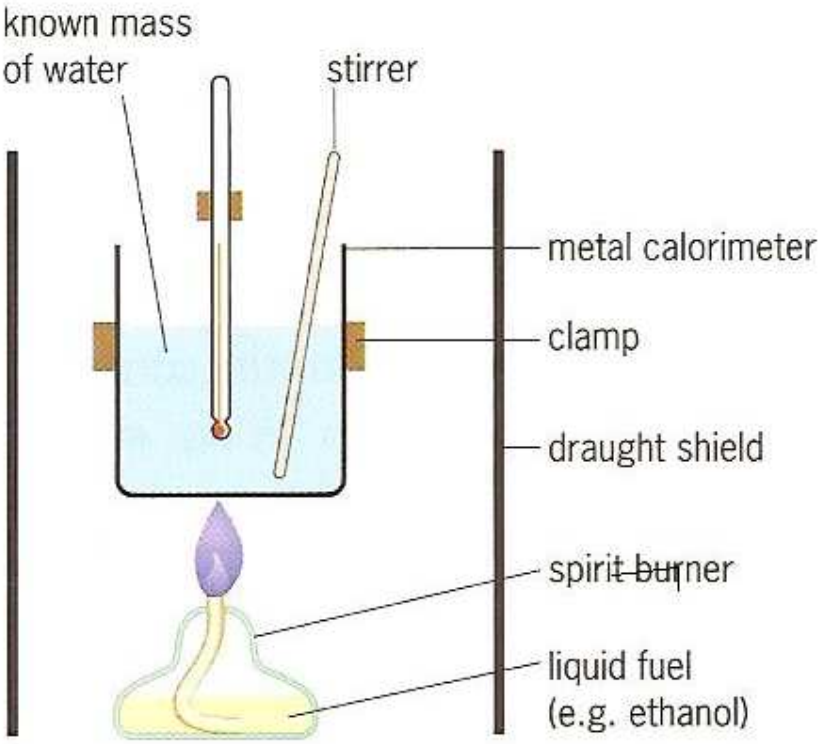
I have completed a preliminary test in my module developing fuels as an activity 1.2. I have experimented using the two fuels methanol and hexan e. My results show that hexane's "1227.8 kjmol^{-1}" enthalpy change of combustion is a lot higher than that of methanol's "387.1kjmol^{-1}"; this is because hexane has many more bonds to be broken down and new ones to be made. This is because, the size of the molecule (hexane) is much larger compared to molecule (methane).

When hexane reacts, all O-H bonds must be made, which gives a more exothermic reaction. Fuels that contain oxygen like methanols are called oxygenate and have lower enthalpy change of combustion.

Diagram

This is the way I will set out my apparatus, which I have listed below.



Equipment

- Copper calorimeter; with a base diameter of at least 10 cm^3. This is where I will put the 200cm^3 of water. The copper is a good conductor therefore it will allow more of the energy to get to the water compared to other metals.
- Clamp stand; this will be used to hold the copper calorimeter right above the flame which will ensure the heat and energy from the flame isn't wasted at all. The clamp stand is the best choice because a metal tripod will heat up itself and energy will be lost.
- Metal stirrer; to stir the heated water in order to get the heat equally dispersed in water.
- Electronic balance; this would weigh the spirit burner to two decimal places which allows higher accuracy when calculating an accuracy.
- Draught excluders; which are tiles put around the ex periment to prevent heat loss and are safer to use as it will help prevent things set on fire.
- Goggles; these would be worn to protect eyes as some fuels are irritant*.
- Measuring cylinder; this will be used to measure 200cm^3 of water, to a good degree of accuracy.
- 0-100°C thermometer; this will be used to measure the waters temperature rise; I have chosen a 0-100°C because it's more accurate.
- Spirit burners containing;
  i. Methanol
  ii. Ethanol
  iii. Propan-1-ol
  iv. Butan-1-ol
  v. Pentan-1-ol

These are the fuels which will be bu rned to heat up the water in the calorimeter.

Method

Firstly I will put on my protective clothing and my goggles because of the dangers explained further on. I will then add the fuels which I will compare; into the spirit burner, which I had alre ady emptied, washed and dried before hand. I will then weigh my spirit burner filled halfway with the liquid fuel. I will place the spirit burner on a heat proof mat for safety in case of any spillages I will then record the weight in my table of results. I will then measure out two lots of 100cm^3 of water using my 100cm^3 measuring cylinder; I will then pour it into the copper calorimeter, I will then place the copper calorimeter into a clamp which will be approximately 10 cm above the mat leaving enough ro om between top of spirit burner and bottom of the cal orimeter for the flame to burn, preventing any heat loss into the air.

I will then place the four draught excluders around the copper calorimeter and spirit burner so they surround the items and pr event heat loss. I will then clamp the thermometer, into the water making sure it doesn't touch the bottom of the calorimeter as it could heat up and skew my results . I will then wait for it to reach waters temperature, when reached; I will record it on my results table.

I will then place the burner under the calorimeter and light the wick. As water is heated, I will wait until a temperature change of 20°C is reached. I will then extinguish the burner and note the mass of the spirit burner with the evaporator lid on the prevent heat loss due to evaporation. I will also note the highest temperature reached. Using the results I have recorded I will be able to work out the temperature change and the change in alcohols mass.

I will use the formula below to calculate heat transferred number of moles and finally the enthalpy change of combustion.

- Heat Transferred> $cm\Delta T\ (X)^2$
- Number of Moles> $N= M/Mr(Y)^2$
- ENTHALPY CHANGE OF COMBUSTION> $(^X/_Y/1000)^2$

I will repeat my experiment three times with each fuel to gain a reliable and concordant set of results. All of these results will record my results in a table as shown below.

ALCOHOLS	START MASS(g)	END MASS(g)	MASS CHANGE(g)	START TEMP(°C)	END TEMP(°C)	TEMP CHANGE(°C)
FUEL1st trial						
2nd trial						
3rd trial						

Safety Precautions

The use of these fuels above may expose me and other s near me to hazards, some of these are; that these fuels are highly toxic, irritant and harmful also highly flammable therefore must be very careful w hen lighting the flame in order to prevent fire[3]. They all have flash point below 21° C and may easily catch fire, I will try and prevent this by using screens, protective clothing and gloves. These fuels above are irritant to the respiratory system and to avoid any damages I will carry out my experiment in a very well ventilated laboratory, near a fume cupboard if possible. There is also a high risk of the fuels getting into eyes in addition to to prevent any damage I will use safety glasses.

Harmful

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Highly Flammable

Fair Test

To enhance a non biased experiment, I will try and keep the confounding variables as low as possible. These include; keeping the rooms condition the same, e.g. ensuring the rooms temperature is the same throughout my experiment, as it coul d skew my results and end up heating the water even more. I will also pay attention to my electric scale, making sure that it works and is accurate each time I weigh my fuel. I will also have to evaluate my results to see if they are concordant and they ar e not very extreme.

Accuracy

To increase accuracy I will make sure that the equipment I use is reliable and the right choice for my experiment. I will use a copper calorimeter and draught excluders to ensure minimum heat loss during the experimen t. I will make sure the electronic scale is programmed to show mass to, two decimal places, which will allow a precise result. I will use a 100cm³ measuring cylinder which I will use twice to reach the 200cm³ water for my experiment, this will ensure that the water is measured to a good degree of accuracy. I will also use a 0-100°C thermometer; again this is to ensure accuracy is met to a good degree.

Analysis

Below is the table of results of the fuels that I've burnt, to find an average enthalpy change of combustion.

FUEL	START MASS (g)	END MASS (g)	MASS CHANGE(g)	START TEMP (°C)	END TEMP (°C)	ΔH ($kjmol^{-1}$)	AVERAGE ΔH_C ($kjmol^{-1}$)
METHANOL 1.)	185.26	183.41	1.85	22	42	-290.59	-255.27
2.)	183.41	181.01	2.4	43	63	-224.00	
3.)	181.01	178.87	2.14	20	40	-251.21	
ETHANOL 1.)	216.20	214.38	1.82	42	62	-424.61	-474.10
2.)	214.38	212.95	1.43	19	39	-540.42	
3.)	212.95	211.26	1.69	39	59	-457.28	
PROPAN-1-OL 1.)	183.54	182.15	1.39	26	46	-725.18	-724.84
2.)	182.15	180.83	1.32	21	41	-763.64	
3.)	180.83	179.36	1.47	24	44	-685.71	
BUTAN-1-OL 1.)	143.83	142.49	1.34	20	40	-927.76	-916.44
2.)	142.83	141.13	1.36	40	60	-914.12	
3.)	141.13	139.76	1.37	18	38	-907.45	
PENTAN-1-OL 1.)	190.95	189.65	1.3	27	47	-1173.33	-1155.28
2.)	189.65	187.39	1.26	47	67	-803.48	
3.)	187.65	185.55	1.84	18	38	-1137.23	
HEXAN-1-OL 1.)	178.10	176.92	1.18	42	62	-1452.20	-1520.48
2.)	176.92	175.87	1.05	18	38	-1632.00	

3.)	175.87	174.71	1.16	41	61	-1477.24	

Using the information I have gathered from my results, I have worked out the enthalpy change of combustion for the six alcohols. Using the formula's I have mentioned previously, these were;

- Heat Transferred> CxMxΔT (X)

C is equal to the specific heat capacity of water it is equal to 4.18, which will raise the waters temperature by one Celsius. M is the mass of water used; in this case it was always $200cm^3$. I have collected three sets of results for each fuel to get reliable and accurate results.

I will run through the calculations for one of the fuels.

The fuel I will use as an example is Methanol. I have kept the temp ri se variable constant meaning my temperature change was always 20°C.

I will use this information and put it into formula to find the ΔH_c for methanol.

Energy > 200 x 4.18 x 20

M x C x ΔT = 16800J

So I can say that the energy transferred was 16800J.

To find out how much energy should have been released for one mole of the fuel; I will firstly get my 1st 2nd and 3rd trials for methanol.

FUEL	START MASS (g)	END MASS (g)	MASS CHANGE(g)	START TEMP (°C)	END TEMP (°C)
METHANOL 1.)	185.26	183.41	1.85	22	42
2.)	183.41	181.01	2.4	43	63
3.)	181.01	178.87	2.14	20	40

I know that methanol; CH_3OH has 1carbon, 1oxygen and 4hydrogen's present in one mole. So to work out the molar mass;

Mr = 12+16+4

Mr = 32g

Now that I know the M_r of methanol I could work out the number of moles, using the formula below.

- Number of Moles> $N = \frac{\text{Mass change}}{M_r}$

1.) Number of moles = 1.85/32 = 0.0578mol

ΔH_c = (16800/0.0578)/ 1000= $-290.59 kjmol^{-1}$

I will use the same technique to get the enthalpy change for my 2 nd and 3rd trials.

Mass change

In order to convert my answer to kJ I will need to /1000

2.) 16800/(2.4/32)/1000 = $-224.00 kjmol^{-1}$

Energy

M_r

3.) 16800/(2.14/32)/1000 = $-251.21 kjmol^{-1}$

To find an average of my results I have then added all of the enthalpy changes I have gained, of all the trials;

$(-290.59)+ (-224.00) + (-251.21)/3 = -255.27\ kjmol^{-1}$

After completing the steps for all of the fuels, I have recorded them on the table above.

Breaking bonds is an endothermic reaction which requires energy to break bonds; but if it takes energy to break bonds it must release energy when new bonds are formed. This reflects the first law of thermodynamics (law of conservation of energy) 'energy can neither be created nor destroyed .'[2]

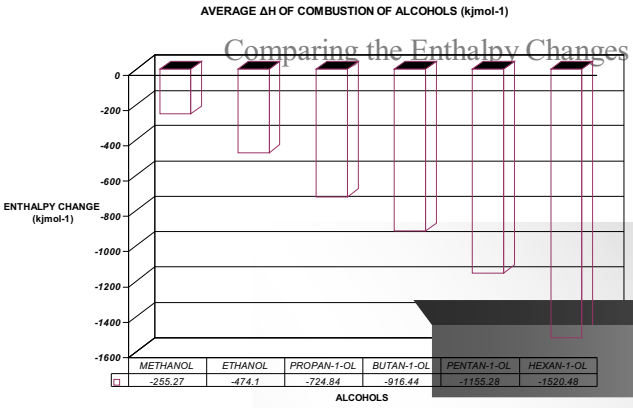
E.g. when methanol burns in oxygen;

$CH_3OH + 1.5O_2 \longrightarrow CO_2 + 2H_2O$

$E(C\text{-}H_3O\text{-}H) + 1.5\ E(O=O) \longrightarrow -E(C=O) + 2 - E(H\text{-}O)$[2]

The energy given off when fuels burn is the difference between the energy required to break bonds and the energy released when bonds are made. There are more bonds in hexan-1-ol than in methanol while this means you need more energy to break bonds in a mole of hexan-1-ol far more energy is released when new bonds are formed with oxygen.

The energy transferred was the same for all the fuels however hexan-1-ol has 14 hydrogen bonds where as methanol has 4 hydrogen bonds to break. Already I could see that hexan-1-ol will require roughly 3.5x more energy as methanol to break all of its bonds.



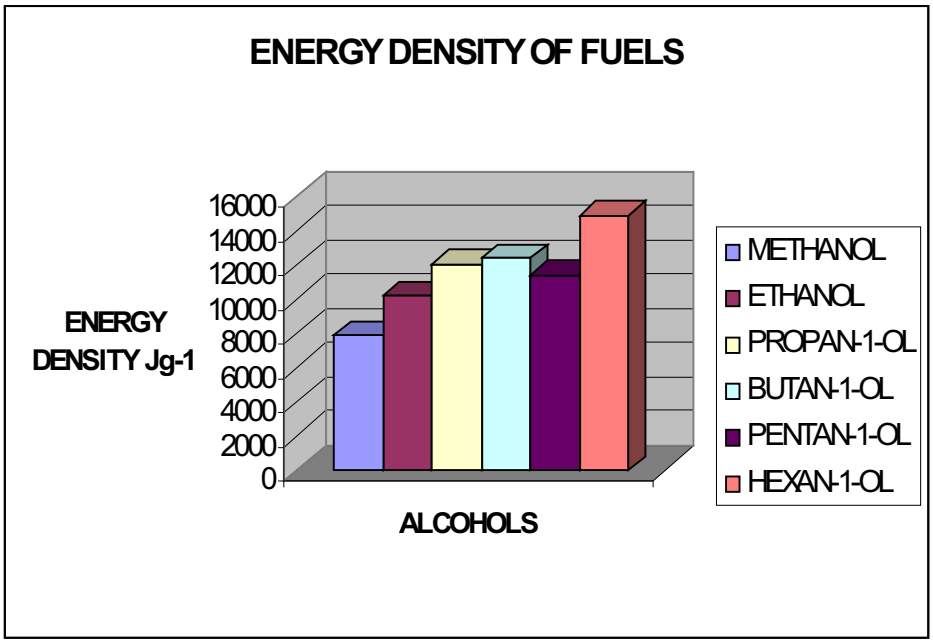
AS THE NUMBER OF CARBONS INCREASE, THE ENTHALPY CHANGE OF COMBUSTION INCREASES.

Energy Density

Most means of transport has to carry their own fuel around with them, e.g. petrol in the tank of a car therefore obtaining the maximum amount of energy from the smallest mass of fuel is v ital. This is called the energy density of fuel. To calculate the energy density I have divided the energy transferred by mass of fuel used; I have got my answer in Jg^{-1}.

ALCHOHOLS	ENERGY DENSITY (Jg^{-1})
METHANOL	7887.32
ETHANOL	10181.82
PROPAN-1-OL	12086.33
BUTAN-1-OL	12352.94
PENTAN-1-OL	11420.57
HEXAN-1-OL	14867.26

As seen from my results hexan-1-ol has the highest energy density meaning it is the most efficient and convenient fuel. The reason why propan -1-ol has a lower energy density than butan-1-ol is because I have not discounted the outlier thus it's skewed. However we could see the general pattern which is; the higher the number of carbons the higher the energy density.



Evaluation

My experiment showed consistent increase in enthalpy change of combustion as more carbons were used the higher its enthalpy change was, therefore it shows the trend expected.

I have tried my best to keep my results accurate by using my calculations to 2.dp. at all times. However I had an outlier on my second trial of pentan-1-ol. This proves that I might have been limited by the accuracy of the measuring cylinders, to measure out twice 100cm^3, however they are the least accurate, as I have only measured from the meniscus point meaning there is at least +or-5cm^3 error. To work out the percentage error, I will determine the graduations on the 100cm^3, in this case its every 10 cm^3, implying that so my error would be 5cm^3 in my reading. Therefore percentage error would be 5/100x100= 5 % however because I have measured 100cm^3 twice this would add up to 10 % altogether.

When calculating a temperature change there is a possible error of +or - 0.5°C at the start and end of temperature change. Therefore the percentage error on my reading on average calculated by;

Start 20°C → 20 +or- 0.5

End 45°C → 45 +or – 0.5 total error = +or- 1.

Therefore my percentage error is 1/25x 100= 4%

There is also a percentage error calculated when using the balances to calculate the mass of fuel. The balance I have used had read the mass to 2.dp. meaning they have readings every 00.1g. Therefore the average percentage error of measuring the mass of fuel is 0.005/1.00x100= 0.5% this percentage error is times by two because the same fuel was weighed twice before and after lighting it up therefore its 1%.

Consequently we could assume that the percentage error on average for the whole experiment can be calculated by adding the sum of all of the individual percentage errors, 1% + 4% + 10%= 1 5% error, as seen from calculations the measuring cylinder has the most percentage error, this is partly because, I had to measure two lots of water from the 100cm^3 cylinder. Therefore to improve the accuracy I could use a burette to measure the volume of water. Burettes have a lower percentage error than that of a measuring cylinder, they have graduations every 0.1cm^3 so when taking a reading it could be no more than +or- 0.05cm^3, which is a lot smaller than that of a measuring cylinder.

There are also many confounding variables such as the draught excluders were fastened by blue tack and not perfect. The convection of heat may have escaped into the surroundings air entering through the gaps and through the top. Incomplete combustion is also a possibi lity which confound with accuracy of the experiment. The incomplete combustion of the fuel would mean the fuel leaving the burner but to produce carbon monoxide and even carbon (soot) would remain unburnt, so when weighing
the burner the incomplete combustion wouldn't be taken into account and the value of the fuel burnt would be too high.

My results also have an outlier I know this because when comparing my results within their repeats, pentan-1-ol showed that on the first trial; enthalpy change of combustion was "1137.23kjmol^{-1}" and on the second trial it was "1232.00kjmol^{-1}" however my third trials showed that enthalpy change of combustion was only "924.00kjmol^{-1}" this is unexpected and therefore counted as an anomalous result. On the other hand when comparing the enthalpy change of combustion of the fuels I can see a steady rise (when the outlier is removed from the average).

On the whole the fuels may not have burned efficiently; this might have an impact when comparing it to the precision errors as it is not possible to calculate an error for incomplete combustion, evaporation or heat loss. However despite all errors I could still make a valuable comparison about the enthalpy change for the homologous series of alcohols. I could see a rise in enthalpy as the number of carbons increase. However the smaller errors may have built up into a large error and may have biased the overall results of my experiment.

Nevertheless I believe my results were accurate and useful in identifying the highest enthalpy within the alcohols. I believe that they were as accurate as I could possibly do them, most errors were inevitable and due to human error.

If I was to redo the experiment I would focus on using better draught excluders and a lid for my copper calorimeter, in order to prevent heat loss as best as I could. I would also consider using another technique to wait for the water to boil, in this case I was waiting for the water to reach 20 °C and then extinguished the wick, whereas if I was to use a set time, e.g. waiting for 1 minute. It would ensure my results were unbiased and more precise. It is also a lot easier to make mistakes using the thermometer; to know when to stop, as it has to rely on human judgement, whereas using a stopwatch would be easier and more accurate.

I will also make sure that I check the percentage errors on my equipment and decide on the ones which have the smallest percentage error and most suitable.

Overall I believe that my experiment succeeded in finding out which alcohol out of the six provided had the highest enthalpy of combustion.

BIBLIOGRAPHY
(References)

[1] http://www.practicalchemistry.org/experiments/measuring -heat-energy-of-fuels,21,EX.html (picture of an exothermic reaction.)
[2] Collins Advanced Science Chemistry (authors; Chris Conoley and Phil Hills) ISBN;0007135971 Pages 168-170 (Chapter 8) (picture of how to set up apparatus, chemical equations)
[3] Hazcards (hazard cards outlining hazards of the fuels I will be using and the risk control strategies of the particular fuels.)
[4] commons.wikimedia.org/wiki/Image:Hazard_X.svg (pictures of hazard warning)

These references have helped me work out my calculation of enthalpy change of combustion, gave me definitions of some words, and gave me drawings of how my apparatus will be set up, and a picture of an exothermic reaction.