

Chemistry Coursework

Comparison of Enthalpy Changes of Combustion of Different Alcohols

Aim: To investigate how and why the enthalpy of combustion of varying alcohols is affected by molecular structure.

The enthalpy change of combustion refers to the amount of energy transferred when one mole of fuel burns completely. This value was obtained by using various fuels to heat water, knowing 4.2J of energy are required to raise the temp of 1g of water by 1°C, using the following method. The enthalpy change of one mole of alcohol can be calculated from the amount of energy the water has absorbed.

Apparatus

Fuel burners and the following alcohols

Methanol (CH_3OH)

Ethanol ($\text{C}_2\text{H}_5\text{OH}$)

Propan-1-ol ($\text{C}_3\text{H}_7\text{OH}$)

Butan-1-ol ($\text{C}_4\text{H}_9\text{OH}$)

Octan-1-ol ($\text{C}_8\text{H}_{17}\text{OH}$)

Copper Calorimeter

Thermometer

250cm³ measuring cylinder

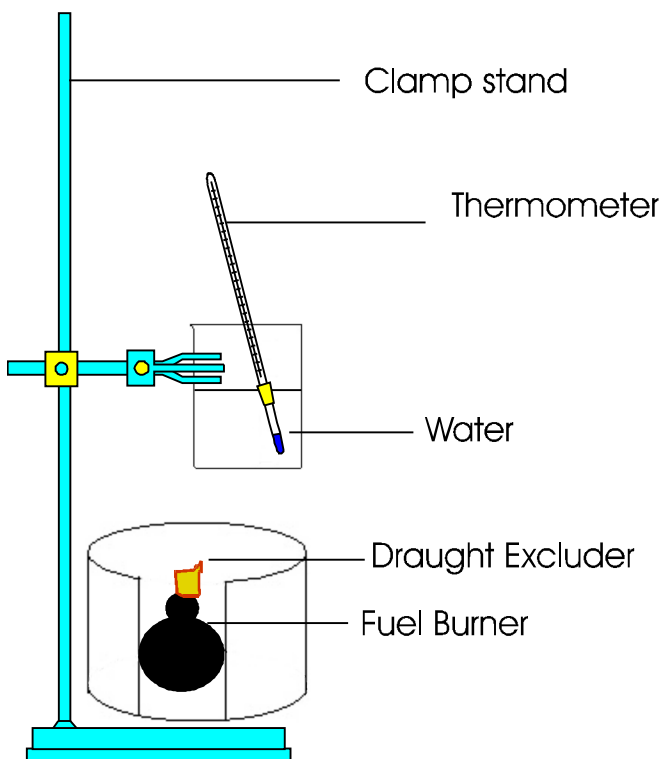
Goggles

Draft excluder

Electronic scales (to 3dp for accuracy purposes)

Stirring rod

Diagram



Method

1. Pour 200cm^3 of water into a copper calorimeter and record the temperature.
2. Using a clamp stand support the calorimeter over your chosen spirit burner. (At this point it is useful to erect some kind of draft excluder, for increased accuracy, in my case I used a tin can.) Any disturbances could affect the infra red radiation being produced by the burning alcohol and help direct it towards the calorimeter.
3. Weigh the burner and alcohol including lid, otherwise the alcohol will evaporate and disrupt the results, record the result in a suitable table.
4. Replace the burner and light wick.
5. Heat the water until it becomes 15°C warmer and extinguish the burner, replace lid, whenever your burner is not in use.
6. Reweigh your burner and lid and record the result.
7. Repeat the experiment with the other alcohol burners keeping each variable the same, record your results. Use the same calorimeter but let it cool down between each experiment; clean off any soot deposits, which could affect the conduction of heat.

I kept the increment of temperature change as constant as possible to prevent the need for unnecessary calculations in arriving at my final enthalpy changes. Due to the extra energy water needs to change state the relationship between the increase in temperature isn't always the same creating an unpredictable curve. An amount of energy will not

cause the 200cm³ of water at an initial temperature of 70°C to the rise as that of 30°C initially.

Risk Assessment

- Wear eye protection
- Be sensible around naked flames, alcohol burners often have flames that are not clearly visible in sunlight.
- Experimental equipment may be hot during and for some time after the experiment, so refrain from touching it before it cools sufficiently.
- Alcohols are flammable, avoid spillages whenever possible.
- Alcohols fumes can be harmful.
- Remain at a safe observing distance whilst carrying out the experiment.
- Long wicks encourage large flames so keep the wick to a minimum.

Accuracy

In an effort to make the experiment a 'fair test' the only variable I will change will be the fuel that I am using, unfortunately the fuel container may differ but this should not affect my results to greatly, and address the following points.

- The last digit of any set of scales is always an approximation when the value has been rounded, hence the need for scales to at least (2dp). When I weigh the bottle of fuel they cannot be more than 0.005 out, which is a negligible amount. A set of scales to any lower accuracy would incorporate substantial error and there would not be a noticeable difference between the final mass and the initial mass.
- The wick must always be the same size no more than 1cm for safety reasons.

I chose to repeat my experiment with each burner twice an average the difference to help ensure my results are more accurate.

Alcohol	Initial mass (g)	Final mass (g)	Difference in mass (g)	Average difference (g)	Initial Temp °C	Final Temp °C
Propan-1-ol	331,308	330,117	1,191	0.9195	21	36
	328,543	327,895	0.648		21	36
Ethanol	228,921	227,927	0.994	0.9735	17	32
	247,798	246,845	0.953		20	35
Butanol	196,142	149,570	46.572	235.355	18	33
	172,171	171,672	0.499		16	31
Octan-1-ol	295,654	204,958	90.696	70.597	23	39
	210,871	151,373	50.498		17	32
Methanol	226,241	225,033	1.208	1.1755	20	35
	225,031	223,888	1.143		19	34

Calculating Enthalpy of Combustion

To define the relevance of the figures above we need to calculate the enthalpy of combustion of each alcohol.

We need to use the enthalpy formula.

$$Q = mc\Delta T$$

c = Specific heat capacity of H₂O is 4.2 g⁻¹ K⁻¹

T = Temperature change is always 15 °C

m = Mass is (density of water being 1.0 cm₃⁻¹) = 200g

This is a typical calculation to determine the enthalpy of combustion of propan-1-ol from my experimental results.

The amount of energy taken in by the water = 200 x 4.2 x 15 = 12600J (12.6 KJ)

To calculate the amount of moles of propan-1-ol were used in the experiment we first need to calculate it's molecular mass.

$$C_3H_7OH = (12 \times 3) + 7 + 16 + 1 = 60g$$

$$1.191g / 60g = 0.01985 \text{ moles}$$

Therefore 1 mole of propan-1-ol will release:

$$12600J / 0.01985 \text{ moles} = 634.707053. \text{ } 634.7 \text{ to } 1 \text{ (dp)}$$

As with all exothermic reactions heat gain by the surroundings must have come from some energy loss in the reaction making the enthalpy a negative figure.

Propan-1-ol in this case is calculated to have an enthalpy of combustion of – 635 (3sf) KJ mol⁻¹.

The following table represents all the relevant enthalpies derived from my experiment, using the same method of calculation. There are two results for each alcohol, which I attempted to average to arrive at a more accurate result.

Alcohol		Energy of combustion n KJ mol ⁻¹	Average energy of combustion KJ mol ⁻¹	Standard Enthalpies kJmol ⁻¹	Difference in KJ mol ⁻¹	Percentage Error
Methanol	A	-334	-343	-726	32.86	53
	B	-353				
Ethanol	A	-583	-595.5	-1367.3	228.2	56
	B	-608				
Propan-1-ol	A	-635	-1167	-2021.0	854	43
	B	-1167				
Butan-1-ol	A	-20	-1869	-2675.6	806.6	31
	B	-1869				
Octan-1-ol	A	-18	-24.86	-5293.6	212.6	99.7
	B	-32				

The next columns compare my results to the standard enthalpies of combustion from each alcohol. Standard conditions refer to

- A pressure of 100 kilo Pascal's (102 KPa)
- A temperature of 298 k (equivalent to room temperature)

Evaluation

Comparing my results to the standard enthalpies of combustion I believe that both in the propan-1-ol and butan-1-ol experiments that the figures in red are anomalous. I make this assumption on the fact that the other values are closer to the expected theoretical figures, so I decided to disregard some of my results and took the better answer rather than an average of the two, although the other figure is not proven to be very accurate.

This can be seen from the percentage error.

Propan-1-ol

$$-635/-2021 = 69\% \text{ error}$$

$$-1167/-2021 = 43\% \text{ error (making this the preferred answer)}$$

Butan-1-ol

$$-20.02/-2675 = 99\% \text{ error}$$

$$-1869/-2675 = 31\% \text{ error (making this the preferred answer)}$$

I would attribute these inaccuracies to the difficulty in regulating wick length and the ineffectiveness of the draft excluder allowing heat to escape – encouraging a less negative enthalpy than expected. A more enclosed draft excluder that would still allow the alcohol to burn efficiently would encourage more accurate results. If the calorimeter was lowered and had a larger surface area at the base less heat would be transferred to the

water instead of the atmosphere improving my results. A possible delay in reading the thermometer may also have caused inaccurate results, substituting a digital thermometer rather than a conventional one may have made the results more reliable in recording the peak temperatures.

Heat may also have escaped through radiation and conduction through the calorimeter and the tin draft excluder. Insulating the calorimeter may reduce this heat loss.

The accumulation of soot on the base of the calorimeter during the experiment delayed the conduction of heat and therefore affected the final result by making the fuel burn longer to heat the water up to the right temperature.

Overall the general accuracy is around 50% the average being 45.75%, ignoring the obviously flawed octan-1-ol experiment. As the octan-1-ol burned more readily than the other alcohols this probably allowed for greater heat loss to the atmosphere. This greater energy could be observed by the relative size of the flame compared to the other alcohols, which did not release as much energy in the given time as octan-1-ol would, although this should not affect the correlation.

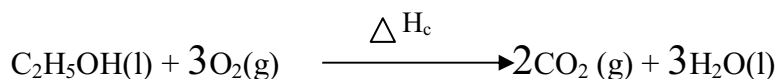
In an attempt to improve my results, if I were to repeat this experiment again, I would certainly examine more alcohols, with higher numbers of carbon chains and increase the number of times I repeated each experiment to improve on accuracy. I would try to use more accurate equipment, under controlled conditions. It may also be an idea to look at isomers of different alcohols propan-2-ol and propan-3-ol for example. Investigation of isomerism should find that these molecules have a less negative enthalpy, due to the side OH group on the alcohol. Which means in regards to enthalpy of combustion they will have a different relationship in to the straight chain ones, due to their molecular structure.

Analysis

Bearing in mind the apparent unreliability of the evidence I collected, relying on one result for two experiments and the overall accuracy not exceeding 69%. I can make the following conclusions. That enthalpy of combustion increases in negativity as you increase the number of carbon in the chain.

To understand why this occurs we must first explain what is happening to the molecules of alcohol when they are burnt.

Take the complete combustion of ethanol for example, where all the C-H and C-C bonds are broken to form the new products carbon- dioxide and water.



The bonds are broken when there is sufficient energy (activation energy) in the alcohol this process takes in energy. New bonds form giving out energy, this exchange of energy

determines the final enthalpy, as all the bonds have specific bond enthalpies. The difference between the sum of bonds broken and the sum of new bonds formed is the enthalpy of combustion. Therefore it is logical to suggest that as you lengthen the carbon chain and add a two more hydrogen molecules each time you will increase the negativity of the enthalpy, within a linear relationship.

Ignoring the obvious anomaly of the octan-1-ol result I plotted a graph (see back page) to represent the enthalpy of combustion for my chosen alcohols. Comparing the two you can see that the theoretical values are more linear which is more expected. To predict the trend for the larger molecules I would suggest that the line would get increasingly steeper as it begins to do in both cases.

Sources

I researched the properties and combustion of alcohols, from a variety of sources including books and the Internet.

Named sources

Ratcliff Brian, Eccles Helen, Johnson David, Nicholson John, Raffan John (2000)
Chemistry 1, Cambridge University Press

Ritchie Rob (2000) Letts Education Revise AS Chemistry, Letts education

Chemistry data Booklet (used to obtain the theoretical enthalpies)