International Baccalaureate

Extended essay cover

SAMPLE B

Diploma Programme subject in which this extended essay is registered: CHEMISTRY

(For an extended essay in the area of languages, state the language and whether it is group 1 or group 2.)

Title of the extended essay: Is there are variation in the amount of caffeine in black teas produced differently, by comparing brands of tea produced by different manufacturers?

Candidate's declaration

If this declaration is not signed by the candidate the extended essay will not be assessed.

The extended essay I am submitting is my own work (apart from guidance allowed by the International Baccalaureate).

I have acknowledged each use of the words, graphics or ideas of another person, whether written, oral or visual.

I am aware that the word limit for all extended essays is 4000 words and that examiners are not required to read beyond this limit.

This is the final version of my extended essay.

Candidate's signature: ______________________ Date: 10/02/2009.

IB Cardiff use only: **A:** 14,736 **B:** ________

International Baccalaureate, Peterson House,

Supervisor's report

The supervisor must complete the report below and then give the final version of the extended essay, with this cover attached, to the Diploma Programme coordinator. The supervisor must sign this report; otherwise the extended essay will not be assessed and may be returned to the school.

Name of supervisor (CAPITAL letters) ____________________

Comments

Please comment, as appropriate, on the candidate's performance, the context in which the candidate undertook the research for the extended essay, any difficulties encountered and how these were overcome (see page 13 of the extended essay guide). The concluding interview (viva voce) may provide useful information. These comments can help the examiner award a level for criterion K (holistic judgment). Do not comment on any adverse personal circumstances that may have affected the candidate. If the amount of time spent with the candidate was zero, you must explain this, in particular how it was then possible to authenticate the essay as the candidate's own work. You may attach an additional sheet if there is insufficient space here.

original idea was very different to this EE. She spent her whole 6 week Summer break collecting data only to find that it did not make any sense at all. To her credit, she changed the focus completely and continued to her practical work. She, therefore, was quite a bit behind her peers but worked hard to complete the essay. ✓ helpful.

I have read the final version of the extended essay that will be submitted to the examiner.

To the best of my knowledge, the extended essay is the authentic work of the candidate.

I spent [5] hours with the candidate discussing the progress of the extended essay.

Supervisor's signature: ____________________ Date: 10/2/2009

0

Research Question

Is there a variation in the amount of caffeine in black teas produced differently, by comparing brands of tea produced by different manufacturers?

Session: May 2009
Candidate Name:
Candidate No.:
IB Subject: Chemistry
Supervisor:
Word Count: 3,969 ✓

Abstract: In this essay I am exploring the effect of the production of tea on its caffeine content, using the question: *Is there a variation in the amount of caffeine in black teas produced differently, by comparing brands of tea produced by different manufacturers?*

The scope was to determine what processes have an effect on the levels of caffeine in tea, if there was an effect. As part of the production, brand, manufacturer and region grown were considered. By *production*, it is meant how the tea leaf on a plant to what is in the average tea bag. By *brand*, it is meant what name the tea is sold as –Ceylon, Darjeeling, Earl Grey. By *manufacturer*, it is meant the company that produces and sells the tea. The amount of caffeine present in each different was found by doing a series of experiments to extract the crystalline white solid, caffeine. From finding the mass of this caffeine, and using the known molar mass – the moles of caffeine obtained from each experiment were compared. This was able to be done as the same mass of tea leaves were stewed for each experiment.

It was found that the manufacturer, Ahmad™, had the most caffeine on average, and the highest value for caffeine was in the Ahmad™ Ceylon tea – with 0.001789 moles ± 0.000005 of caffeine per gram. There was no consistent pattern between different regions, Ceylon and Darjeeling teas – with Ceylon tea having about 0.00050 moles ± 0.00001 more than Darjeeling for Ahmad™ and having 0.00105 moles ± 0.00001 less than Darjeeling for Dilmah™. There was no tea that had an overall greatest value, with Darjeeling tea the most consistent, in caffeine, between the two manufacturers. In conclusion, there is a variation in caffeine due to how tea is produced.

Word count: 297

Contents Page

Introduction

Why I chose this topic?

When choosing a question, I decided I wanted to do something that would apply to my everyday life. I felt I would have achieved something and see things differently, day to day. Tea has long been seen as some British thing, and having a grandmother and mother who both love it, it was a tempting topic. Also, having been on a trip to India, where the choice was so varied, and living in a region where there are so many different types of tea available, it seemed reasonable. As I had heard of many extended essays with titles relating to the finding of the levels of caffeine between black, oolong, green and white teas, I was reluctant to go down this route. As well as this, I also thought that there was much more to the production, how the tea leaf on a plant to what is in the average tea bag, than just these four types, with black tea being the basis of many major teas (such as the ones I chose in my experiments). I thought it would be interesting to directly compare brands – what name the tea is sold under (for example: Ceylon, Darjeeling, Earl Grey) and the preparations of the same tea leaf (in my case, the black tea) to see on an even smaller scale, if there were any variations in the moles of caffeine when a cup of tea was made. Essentially there is only one type of tea leaf, and hundreds of different types can be made from it. Focusing on one area of all of this seemed to be the most logical option. And so I came up with my question: *Is there a variation in the amount of caffeine in black teas produced differently, by comparing brands of tea produced by different manufacturers?* otherwise much too broad.

Approach

I approached this question by first deciding what I wanted to test. Through research, I found that out of the four basic types of tea leaves, the black, green, white and oolong (as mentioned above), were *not* different species and were merely produced differently to give the final product. The most available to me was black tea. It is contained in various teas such as Earl Grey tea, English breakfast tea, Ceylon tea, Kenyan tea, Darjeeling tea and so on. It became apparent, that the leaves were from different regions, so grown differently. I then chose three teas, each with their own distinction from the other:

- Earl Grey Tea: fundamentally, Ceylon tea, grown in Sri Lanka, with flavouring added, called bergamot, giving it its distinctive taste.
- Ceylon Tea: tea grown in Sri Lanka, with nothing else added.
- Darjeeling: tea grown in northern India, with nothing else added.

This gave me leeway to compare the Ceylon and Darjeeling for how they are prepared or grown in different regions, and Ceylon and Earl Grey to see how the preparation of the tea leaves from the same region effect the caffeine levels. I wanted to see determine whether these differences were consistent between manufacturers, the company that produces and sells the tea , I chose two manufacturers, allowing me to refine my question further, exploring the following factors within the 'preparation':

- how different preparations, or growth factors, compare between regions*
- how different preparations vary the caffeine content with the same tea leaf from the same region*

- how the variations are the same between different companies who make the tea*
**with the assumption that there WILL be some variation*

Along with this, I also tested each tea from each company, three times, to show that the results were standard between each.

Investigation

Background Information

Tea itself is grown as a plant - *camellia sinensis*- whose leaves and leaf buds are processed using several methods to give the final product of the dried tea leaves that are commercially used to use in drinks. There are two variations to this plant based on where they are naturally occurring – *Camellia sinensis var. sinensis* (China tea) and *Camellia sinensis var. assamica* (Assam tea, Indian tea). All types of tea come from this plant – the types being black, green, white and oolong tea. Essentially – they *are not* different tea leaves, they are the same plant's leaves processed differently.

Out of the four, black tea is fermented the longest – the full process that black tea undergoes can be seen in the diagram below.

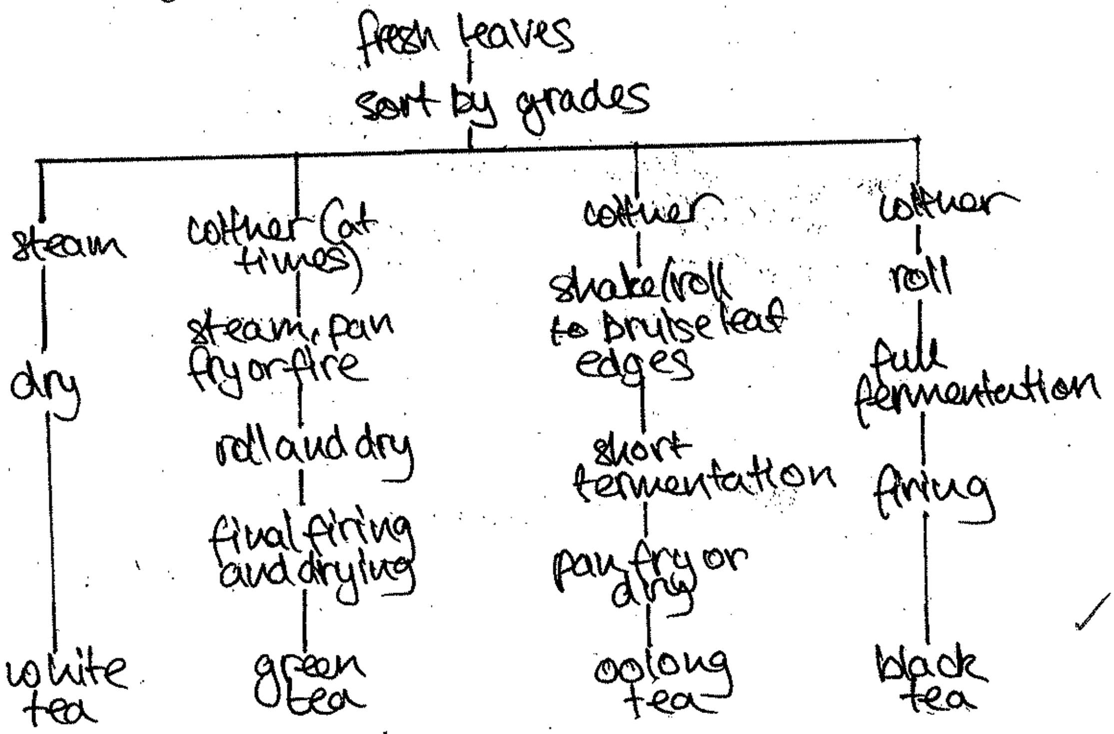


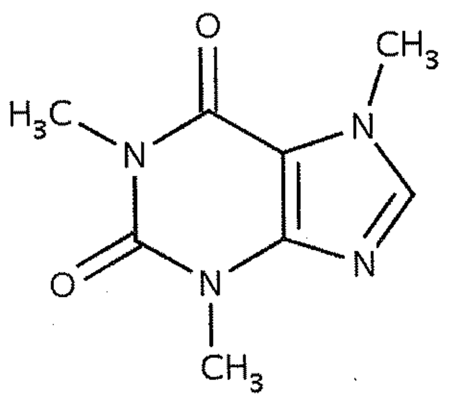
Figure 1 – Diagram of how tea is produced[1]

Withering is started when the leaves are pluck from the plant, and is the natural process of the leaves beginning to decompose. The leaves are spread out where they are left to wither in the sun. They quickly loose water and become limp. The leaves are then rolled and bruised to "break open their leaf cells". They are then in a warm place to ferment. The breaking of their structure and heat encourages reactions within the leaf, as later described – leading to fermentation. The leaves are then heated, or fired, where they are heat to high temperatures and dried. This is the final product that ends up sold commercially.[2]

[1] http://www.planet-tea.com
[2] All information from this paragraph was seen at: http://www.siu.edu/~ebl/leaflets/tea.htm

It is suggested by numerous sources that during the fermentation process the enzymes in the leaf breakdown the tannins and oils in the leaf. This is the stage where caffeine appears to be produced through the action of the catalysts. One source even states that the caffeine undergoes "oxidation"[3]. However, despite an extensive search, the precise reaction of what substance is made into caffeine is not available.

There does appear to be some information – but much of it is published data. However, what is suggested by what was seen was that a structurally similar chemical, theobromine is one of those that leads to the formation of caffeine. It has a similar structure, as seen below in **Figure 3 and Figure 4**, and it also said to be an "alkaloid", a substance that is highly reactive and biologically active at low temperatures.[4] The nitrogen based compounds are the stimulants in numerous illegal drugs – and are the cause for the effect they have on a person.



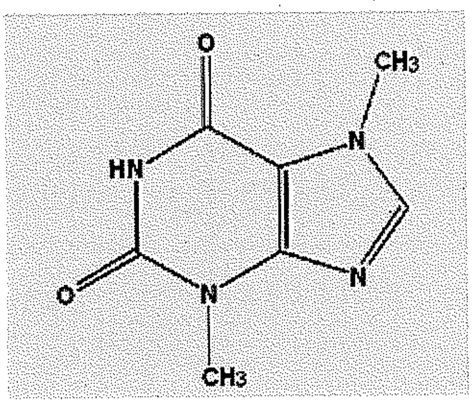


Figure 3: Structure of a caffeine molecule[5] **Figure 4 – the structural formula of Theobromine**[6]

Although complex, the principles behind this reaction are relatively simple. Enzymes, which are catalysts, are activated at certain energies. Activation energy is the minimum energy required for a certain reaction to occur. The enzymes lower the energy for this complex reaction, taking organic materials and making them into caffeine, to occur at. During fermentation, with elevated temperatures, the reaction is more likely to occur – as more molecules will have the correct activation energies, according to the Maxwell-Boltzmann distribution curve, which is a model that shows the effect of raising temperature on a reaction, and whose area under the graph is the number of molecules present in the given reaction.

---

[3] http://www.thefragrantleaf.com/blacktea.html

[4] http://www.friedli.com/herbs/phytochem/alkaloids/alkaloid1.html

[5] http://www.bmrb.wisc.edu/metabolomics/standards/caffeine/lit/9684.png

[6] http://www.phytochemicals.info/phytochemicals/theobromine.php

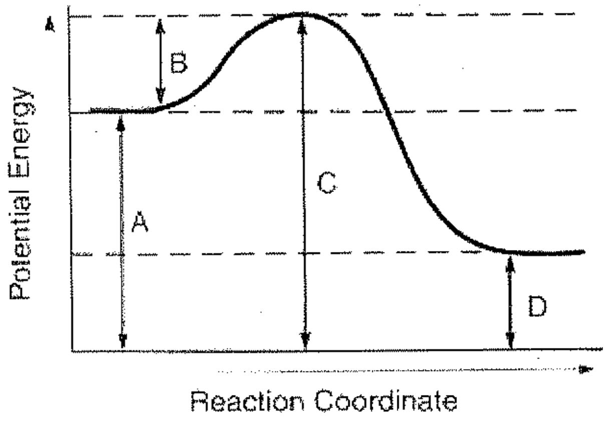


Figure 5 – Energy diagram (with C indicating what is meant by the activation energy for a reaction)[7]

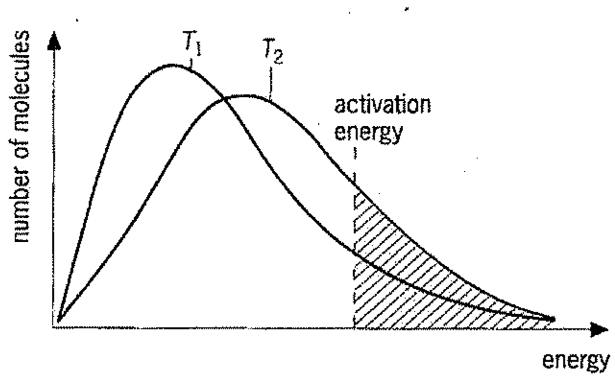


Figure 6 –Maxwell-Boltzmann distribution curve (with T1 being the lower temperature)[8]

the relevance of all this is not clear

very disjointed in places

The initial withering and rolling of the tea is expected to play a part. As the leaves and their cells are a said to be "broken" down. How effectively this is done may play a part in the later processes.

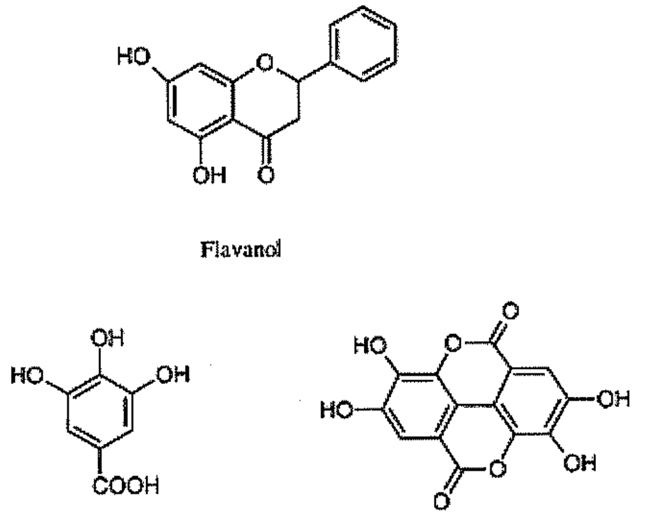
It is also suggested that changing the region of where the tea is grown has some effect on caffeine levels. This is due to two reasons. Firstly – as there are slight variations in the tea plant between regions, the way in which the different types may have adapted to their climate over the years may vary how much caffeine is present. Secondly, the soils in the regions may vary the way in which the plant has grown. Both factors could increase or decrease the amount of caffeine as the plants may act differently and be more susceptible to producing caffeine.

Caffeine itself is a stimulant used in everyday life, with the molecular formula ($C_8H_{10}N_4O_2$)[9]. Figure 3 above shows the structure of the molecule. At room temperature, caffeine is a white,

[7] http://www.chemcool.com/regents/kineticsequilibrium/aim4.h9.jpg
[8] http://www.webchem.net/images/kinetics/wpe1.jpg
[9] http://en.wikipedia.org/wiki/Caffeine

needle-like solid. It has a boiling point of around 178 °C[10] , where is sublimes from a solid to a gas. Its melting point is at 237 °C (when superheated)[11]. Its solubility in water is 22 mg·mL^{-1} at room temperature, and this raises to around 670 mg·mL^{-1} at 100 °C[12]. It is also highly soluble in organic liquids. Tea itself is known to contain around 30mg to 90 mg of this drug, depending on how it is grown, processed and brewed. ref for this?

As mentioned previously, during fermentation, tannins and oils are broken down. Tannins are organic polymers, polyphenols, with their monomer units being simple types of acid, such as gallic acid, or "flavanoids", such as flavanol[13]. Examples of the monomer units can be seen below in **Figure 7**, however the in depth differences between the two types is irrelevant to the investigation as both are present in tea and act in the same way during the experiment. It is worth noting though, that the two variations have differences in their structure leading differing chemical properties, with the condensed tannins being harder to analyse. The two variations are known as hydrolysable and non-hydrolysable, or condensed tannins. ??



Flavanol

Gallic acid M = 170 g mol^{-1} Ellagic acid M = 302 g mol^{-1}

Figure 7: Repeated Units of Condensed Tannins[14]

A very rambling 'introduction' with pieces taken from wikipedia but not in any proper logical or chemical order

[10] http://en.wikipedia.org/wiki/Caffeine
[11] http://en.wikipedia.org/wiki/Caffeine
[12] http://en.wikipedia.org/wiki/Caffeine
[13] http://www.herbs2000.com/h_menu/tannins.htm
[14] Adapted from http://www.rsc.org/ej/AN/2001/b104584a/b104584a-f1.gif

Brief Method [for full look in Appendix III – p.27-28][15]

1. Boil water, then add tea leaves, about 2g which is almost equivalent to an average tea bag, to the water and allow to stew.
2. Using a suction filter, remove the tea leaves and add the sodium chloride.
3. Heat the mixture on the Bunsen burner.
4. Add calcium hydroxide – these chemicals are used to help remove solid and metal ion impurities (such as dust from tea bags) that may be in the solution.
5. Gently place this into the ice bath and leave to cool.
6. Once cool, use the suction filter to remove the precipitate formed.
7. Pour this into the separating funnel and add propan-1-ol.
8. Mix this and allow it to separate out. Pour off the propan-1-ol mixture into a clean flask –repeat this step again.
9. The caffeine and tannins should now be almost all dissolved in the propan-1-ol. Organic material easily dissolves in the propan-1-ol, due to the idea that like dissolves like. Although the water which the caffeine and tannins are already dissolved in is highly polar, there is a large difference in the intermolecular forces between the molecules. Therefore, when the propan-1-ol is introduced, with more similar intermolecular forces in comparison to the water, the tannins and caffeine are easily attracted to the propan-1-ol, as the intermolecular forces between the water molecules is greater than the attraction between the water and the caffeine and tannins. Therefore, the organic materials in the tea are dissolved into the propan-1-ol, leaving behind the water and any other impurities.
10. Then add the propan-1-ol mixture into the separating funnel with the sodium hydroxide. Mix and allow to separate. In this case there is a chemical reaction occurring – where the tannins, which are acidic, undergo a complex acid-base reaction with the sodium hydroxide, producing a salt that is dissolved into the water (from the original 2.5M sodium hydroxide solution). The caffeine does not undergo this reaction as it is not acidic.
11. Pour the propan-1-ol and caffeine mixture into a clean conical flask.
12. Add anhydrous sodium sulphate and swirl with the propan-1-ol mixture, until the sodium sulphate is free flowing (when all water should be removed). The chemical is a commonly used drying agent[16] and is used in such a way in the experiment – to remove any water that may be left over from the previous experimental procedures.

---

[15] Adapted from UWCSEA extraction of caffeine practical (revised June 2008)
[16] http://www.vias.org/genchem/inorgcomp_sodiumsulfate.html

The addition of water lead to it becoming soluble in the water, which is seen when it is described as 'free flowing'.

13. Pour the mixture into a round bottom flask and distil the solution, which removes even more of the water that may remain, further purifying the sample.

14. Pipette 5 ml off into a clean, pre-weighed, Petri dish and leave overnight. Why 5 ml?

15. Once the propan-1-ol has evaporated (a white solid should be observed) add some propanone and leave overnight. The propanone, which has lower melting and boiling points than propan-1-ol, quickly evaporates[17]. The more volatile liquid then attracts any remaining propan-1-ol so leaving pure caffeine behind.

16. Weigh the Petri dish again and compare the differences in mass to find the moles of caffeine that have been produced.

how pure does this method give

[17] http://ptcl.chem.ox.ac.uk/~hmc/hsci/chemicals/propanone.html
http://en.wikipedia.org/wiki/Propan-1-ol

Results

Table of Processed Data

? This is just ½ of the preceeding table

	***Average mass of caffeine per two grams* ± 0.2mg**		***Average mass of caffeine per gram* ± 0.001g**		***Average number of moles of caffeine per gram* ± 0.000005 moles**	
	Ahmad™	Dilmah™	Ahmad™	Dilmah™	Ahmad™	Dilmah™
Ceylon tea	69.3	20.6	0.347	0.103	0.001789	0.000531
Darjeeling tea	43.7	61.4	0.219	0.307	0.001129	0.001582
Earl Grey tea	64.3	17.3	0.322	0.087	0.001660	0.000448

- Ahmad™ and Dilmah™ are the names of the manufacturers used for the tests

- as 2g of tea leaves were used in the experiment, this was about equivalent to one tea bag, or an average cup of tea, therefore mass in mg was left so as to be compared to the range of literature values available, later in the essay ✓

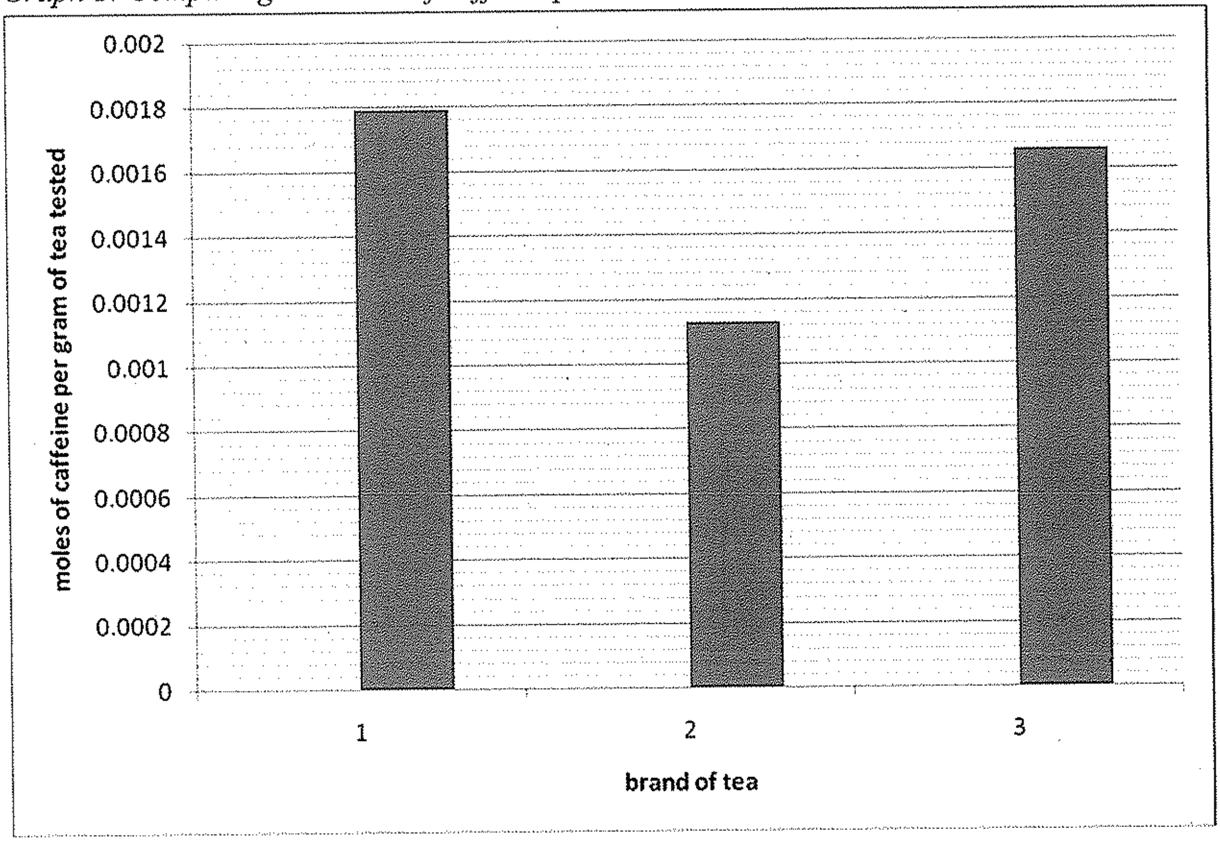
Tables of Raw Data can be found in Appendix's V and VI – p.30 and p.31

Sample Calculation from Raw Data to Processed Data – using the values from Ahmad™ branded Ceylon tea - can be found in Appendix VII – p.32-33

Graphs of Processed Data and Analysis

To compare the results obtained for the moles of caffeine in each trial, the graphs of the results for each manufacturer were compared, and then to show any variation between the manufacturers themselves, the values of each Ceylon, Darjeeling and Earl Grey teas were plotted next to one another to directly compare them. All values used are from the *Table of Processed Data* on p.12: Average moles of caffeine in each tea.

Graph 1: Comparing the moles of caffeine present in Ahmad™ manufactured tea

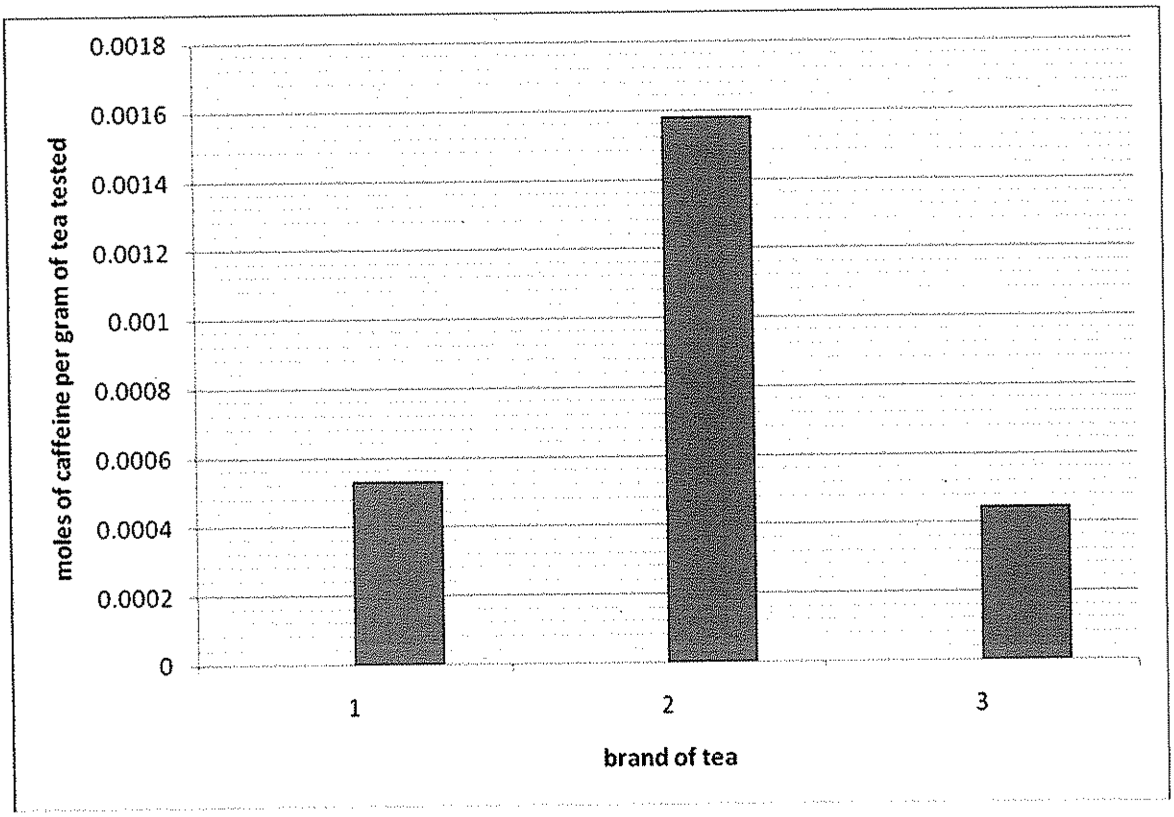


1 – Ceylon tea
2 – Darjeeling tea
3 – Earl Grey tea

Analysis of Graph 1:

It can be seen in *Graph 1* that the Ceylon and Earl Grey teas clearly have much more caffeine than the Darjeeling, about 0.0005 moles more (value from *Graph 1*). This indicates that the region in which the tea was grown played a significant role in how much caffeine was in the tea. It can also be seen that the Ceylon has a little more caffeine than Earl Grey, by about 0.00012 moles – this suggests that Early Grey (due to how it was processed with its additional bergamot flavouring) has been effected by how it was produced – as both teas are grown in Sri Lanka. This shows that region plays a large role in the amount of caffeine.

Graph 2: Comparing the moles of caffeine present in Dilmah™ manufactured tea

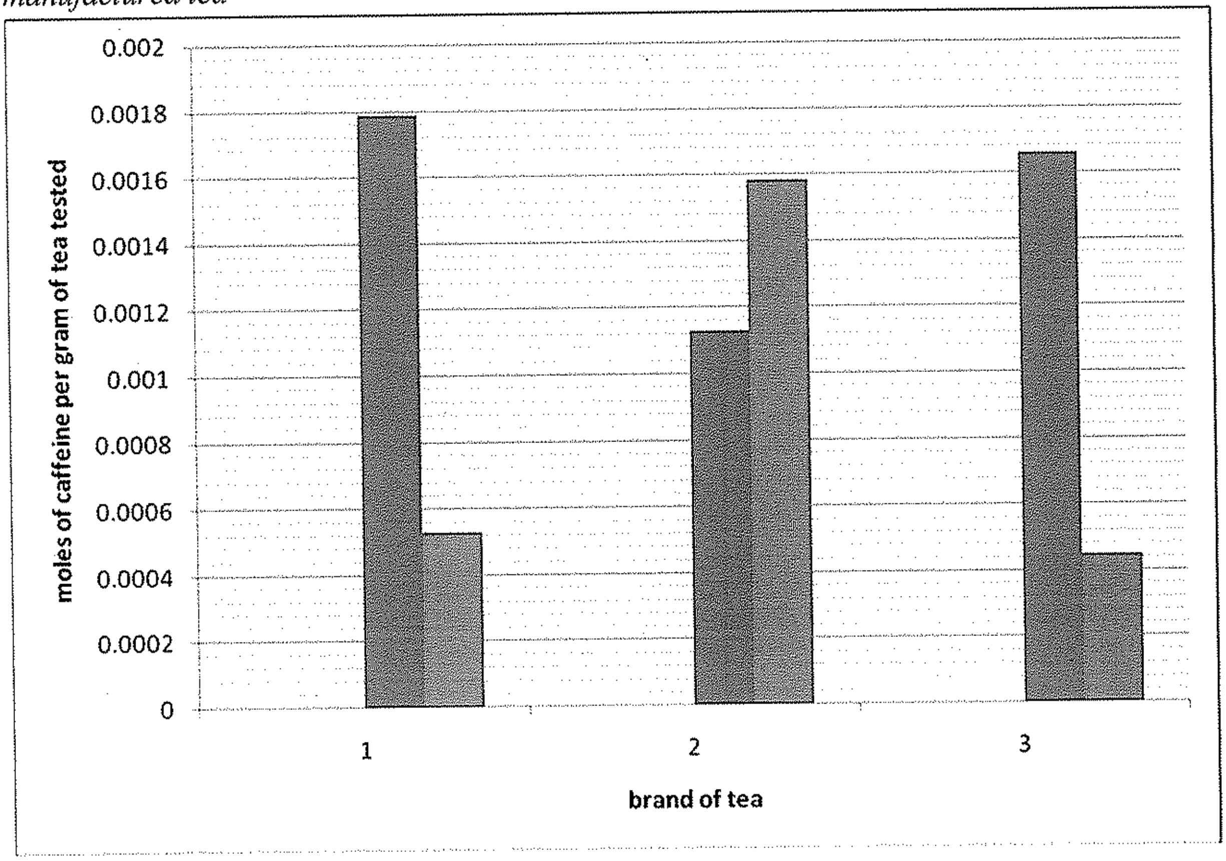


1 – Ceylon tea
2 – Darjeeling tea
3 – Earl Grey tea

Analysis of Graph 2:

The trend of *Graph 2* is different to that of *Graph 1*, on p.13, as Darjeeling now has much more caffeine when it is from the Dilmah™ manufacturer. This shows again, however, that region still plays a great role in the levels of caffeine, with Darjeeling at about 0.00158 moles and Ceylon only around 0.00072 moles (values are from *Graph 2*). There is, again, a higher value for Ceylon than Earl Grey, with a difference of about 0.00028 moles, which is similar to that seen on *Graph 1*, p.13. This reconfirms the idea that the production difference of the addition of flavouring to the Earl Grey has played a role.

Graph 3: Comparing the moles of caffeine present in both Ahmad™ and Dilmah™ manufactured tea



1 – Ceylon tea
2 – Darjeeling tea
3 – Earl Grey tea

Blue - Ahmad™
Red - Dilmah™

Analysis of Graph 3:

It can be seen that the manufacturers must vary their methods of production in some way as there are great difference between the values obtained for Ceylon and Earl Grey teas. The Darjeeling is more consistent – with a difference of about 0.00046 moles between the two manufacturers, in comparison to around 0.00126 moles in the Ceylon teas (values taken from *Graph 3*). On the whole, it can be seen that the Ahmad™ teas have a greater amount of caffeine. The data clearly suggests that there is variation between manufacturers and suggests they must have different ways in which they produce their teas.

Analysis of the Anomalies:

Highlighted in blue on the *Tables of Raw Data* in Appendix V and VI (p.30 and p.31) the anomalies are distinctly lower than the other values obtained for the different trials of the teas. The likely cause of the data being so much lower is experimental error – the trials when being done had many problems and were some of the first two to be done. For example, one had the issue of little propan-1-ol separating out earlier in the experiment, so when the distillation took place, there was just barely sufficient propan-1-ol to put into the Petri dish, which was also likely to be lacking in caffeine due to the fact that little caffeine would have dissolved into the alcohol earlier in the experiment.

✓ Experimental error is the probable reason

Conclusion

In relation to the question: *Is there a variation in the amount of caffeine in black teas produced differently, by comparing brands of tea produced by different manufacturers?* The results of the experiment show that there are clear variations between how what is essentially the same tea leaf has been produced.

The general observations were that, within Ahmad™, the moles of caffeine in the teas grown in Ceylon was much higher than the Darjeeling tea. Within Dilmah™, the moles of caffeine in the teas grown in Ceylon were much lower than the Darjeeling tea. These results suggest that within manufacturers – the place in which tea is grown does play some role. This agrees with the research, which suggests that teas grown in different regions would have different caffeine contents.

For both manufacturers the Ceylon tea also had slightly greater moles of caffeine than Earl Grey, perhaps due to the fact that some of the 2g of tea leaves used were actually the bergamot flavouring from the Earl Grey's production. This also agrees with the research as changing production will change the caffeine content.

The Ceylon and Earl Grey teas, grown in the same region had large differences in moles between the two manufacturers, suggesting that the manufacturers produce the same brands of tea differently, contradicting research, as the processes should be consistent between each manufacturer.

From the experiment, it can be seen that the different factors in the production of caffeine have different effects and can be ranked according to the experiment, in the following manner:

1. *Who the manufacturer is* – must spend longer at different stages during production, perhaps longer time for fermentation.

2. *Where the tea is grown and produced* – the difference in moles between the teas grown in Sri Lanka (Ceylon and Earl Grey) and India (Darjeeling) were not consistent between manufacturers, but were great. This is most likely due to how the tea was grown – affecting the abundance of the organic molecule that is changed into caffeine during the production process. Also, the production may be slightly different between the two regions.

3. *The production between brands of tea (between Ceylon and Earl Grey)* – there is a small difference between the two – as suggested previously, this is due to the fact that bergamot was added to the Earl Grey, directly linked to the production of the tea.

[With 1 having the greatest effect on the moles of caffeine.]

Reliability of Results:

The reliability of the results is high. There is consistency between each trial, with the exception of the two anomalies, which were discussed earlier in the **Analysis** (p.15-16). It can be seen that the errors of the experiment are also relatively low, showing accuracy in the experiment as well. The change in mass of the samples lies within the mass (in mg) of caffeine expected in an average cup of tea, around 30 mg to 90 mg[18], showing a further consistency not only within results, but with other sources.

Related questions/Further research:

From the defining of my research question, to my background research, and throughout my experimentation and analysis, it was apparent that the scope of what I have done during this essay could have been much wider.

Due to the lack of information about what exactly occurs during each step of tea production it would be interesting to go investigate what caffeine content in the leaves is in each stage of production or to do some in depth report of what is done during production, and which steps vary between brands and manufacturers.

Also, as fermentation is often suggested to be the stage in which tannins and different oils are meant to be acted upon by enzymes, it is often assumed that this is the step that affects the caffeine content. It would be interesting as green tea, from previous research, does not undergo fermentation, is actually said to have one of the highest caffeine contents of all four types of tea.

If the caffeine is in fact formed due to the presence of tannins, then a worthwhile investigation might be to see whether the age of the tea leaf – in how long it is left to decompose before it undergoes the production process – affects the caffeine content, hence showing whether there is a link between caffeine and tannins.

Finally, more extensive research into each brand, each manufacturer and each type of tea (green, white, black and oolong) would allow for all steps in more differently produced teas to be assessed.

[18] Based on various sources – listed in the **Bibliography** on p.20

Evaluation

As discussed in the **Conclusion** on p.17-18, the experiment went well on the whole, with only two main anomalies – most likely due to where the experimental procedure went wrong. This plays a key factor in the results – as it does with many results – but particularly as there are many steps, and so many things may go wrong. Some of the problems that arose are listed below, and the solutions (either what *was* done or what should be done in future experiments of this nature):

Problems	*Improvements*
It was not tested whether what was obtained was caffeine. The product looked white and needle-like, as expected, but it was not verified.	Would need to test its melting point or solubility to see if it corresponds to what is expected in research done.
It was difficult to tell whether the caffeine was fully dissolved by the propan-1-ol – as in some cases the propan-1-ol that was separated out was less than that put in originally. To make results fair, little could be done during the experiment to change this, and this effect was only seen a few times – and likely have affected the anomalies in the experiment, as if there was less propan-1-ol obtained, then it is likely that it follows that less caffeine was obtained – thereby effecting the final outcome of the moles of caffeine in the tea.	In future experiments a more effective organic liquid, such as ethoxyethane[19], could be used to dissolve the caffeine (however the safety of its use may have to be determined). One example of a good way in which to dissolve the caffeine is liquid carbon dioxide, which is also used in the commercial decaffeination of drinks, to make them caffeine free[20], however this would need much more specialised equipment and different conditions (pressure and temperatures) to be achieved.
The experiment was long and time consuming – although what was being done was not particularly hard, it was not possible to finish one trial in one day as the distilled propan-1-ol and propanone had to both be left overnight to evaporate. Before the final weight of caffeine could be obtained	Use equipment to help evaporate the organic liquids used and obtained the caffeine more efficiently[21] - in National University of Singapore a complex piece of equipment was used to evaporate the water and extract the caffeine in minutes as opposed to days.
There were still impurities when the propan-1-ol and caffeine mixture were put into the round bottom flask – due to the free flowing anhydrous sodium sulphate that was present after having removed the water. As it was difficult to leave only this material behind without effecting the results – some was added into the distillation process and may have led to the caffeine obtained not being completely pure	Filter out the sodium sulphate left before the distillation process, or pour the propan-1-ol off more efficiently so as to leave the sodium sulphate and water in the conical flask.

yes!

[19] Chemistry For Advanced Level Third Edition by Ted Lister and Janet Renshaw
[20] Chemistry For Advanced Level Third Edition by Ted Lister and Janet Renshaw
[21] Similar method to Bristol ChemLabS method used in their booklet for National University of Singapore course – December 2007

Bibliography

Websites:

http://www.about-tea.com/2005/11/the_four_types_of_tea_1.html	**Publisher not available**	Last Viewed: 18th September 2008
http://antoine.frostburg.edu/chem/senese/101/consumer/faq/decaffeinating-coffee.shtml	**Copyright © 1997-2005 by Fred Senese Comments & questions to fsenese@frostburg.edu Last Revised 07/31/07.URL: http://antoine.frostburg.edu/chem/senese/101/consumer/faq/decaffeinating-coffee.shtml**	Last Viewed: 6th October 2008
http://dictionary.reference.com/browse/caffeine	**Copyright © 2008, Dictionary.com, LLC. All rights reserved.**	Last Viewed: 18th September 2008
http://www.encyclopedia.com/doc/1E1-calciumh.html	**Author not available, CALCIUM HYDROXIDE., The Columbia Encyclopedia, Sixth Edition 2008**	Last Viewed: 6th October 2008
http://www.friedli.com/herbs/phytochem/alkaloids/alkaloid1.html	***Georges-Louis Friedli, PgDip., MSc., CH(t)., MACN., PhD. drfriedli@friedli.com*** ***Last Updated September 1996***	Last Viewed: 6th October 2008
http://www.herbs2000.com/h_menu/tannins.htm	**©2002-2008 herbs2000.com**	Last Viewed: 6th October 2008
http://www.planet-tea.com	**Publisher not available**	Last Viewed: 6th October 2008
http://www.plantcultures.org/plants/tea_production__trade.html	**Copyright is owned in different parts of this website, as follows:** **Website design and all content, except as stated below: Board of Trustees of the Royal Botanic**	Last Viewed: 6th October 2008

	Gardens, Kew. **Images and associated captions: the relevant image partner.** **Stories and associated images and captions: the relevant outreach partner and/or the story contributor.**	
http://www.phytochemicals.info/phytochemicals/theobromine.php	**All content of phytochemicals.info, including text, graphics, logos, is the property of Top Cultures, and is protected by Belgian and international copyright laws.**	Last Viewed: 6th October 2008
http://ptcl.chem.ox.ac.uk/~hmc/hsci/chemicals/propanone.html	***Oxford Coordinator:* Hugh M Cartwright** ***Oxford, May 11, 2006***	Last Viewed: 6th October 2008
http://www.scienceteacherprogram.org/chemistry/Paul00-2.htmlv	**Publisher not available**	Last Viewed: 6th October 2008
http://www.siu.edu/~ebl/leaflets/tea.htm	***Southern Illinois University Carbondale / Ethnobotanical Leaflets /*** **URL: http://www.siu.edu/~ebl/** **Last updated: 3-Oct-99 / du**	Last Viewed: 6th October 2008
http://www.thefragrantleaf.com/blacktea.html	**© Copyright 2002-2007 The Fragrant Leaf LLC. All Rights Reserved.**	Last Viewed: 6th October 2008
http://www.thefragrantleaf.com/teaplanandte.html	**Copyright 2002-2007 The Fragrant Leaf LLC. All Rights Reserved.**	Last Viewed: 6th October 2008
http://www.vias.org/genchem/inorgcomp_sodiumsulfate.html	**Author: Hans Lohninger** **Last Update: 2007-Sep-12**	Last Viewed: 6th October 2008
http://www.wisegeek.com/what-is-theobromine.htm	**Written by S.E. Smith** **copyright © 2003 - 2008 conjecture corporation**	Last Viewed: 6th October 2008

Wikipedia sources:
Pages visited (with dates of when last viewed):

http://en.wikipedia.org/wiki/Acetone	Last Viewed: 29th September 2008
http://en.wikipedia.org/wiki/Caffeine	Last Viewed: 5th October 2008
http://en.wikipedia.org/wiki/Calcium_hydroxide	Last Viewed: 29th September 2008
http://en.wikipedia.org/wiki/Camellia_sinensis	Last Viewed: 5th October 2008
http://en.wikipedia.org/wiki/Propan-1-ol	Last Viewed: 29th September 2008
http://en.wikipedia.org/wiki/Sodium_chloride	Last Viewed: 29th September 2008
http://en.wikipedia.org/wiki/Sodium_hydroxide	Last Viewed: 29th September 2008
http://en.wikipedia.org/wiki/Sodium_sulfate	Last Viewed: 29th September 2008
http://en.wikipedia.org/wiki/Tannin	Last Viewed: 5th October 2008
http://en.wikipedia.org/wiki/Tea	Last Viewed: 5th October 2008

Publisher: **various – not available as it is open for change at any given time by any member of the public – is a secondary source and had to be used due to lack of availability of other resources – primary sources are referenced at the end of webpage.**

Online research papers (abstracts only):

http://www3.interscience.wiley.com/journal/113322134/abstracthttp://www.people.vcu.edu/~asneden/alkaloids.htm	Copyright © 1999-2008 **John Wiley & Sons, Inc.** All Rights Reserved.	Last Viewed: 6th October 2008
http://www.megaessays.com/viewpaper/	All papers are for research and references purposes only!	Last Viewed: 6th October 2008

88685.html	Copyright (c) 2001-2008 **Mega Essays LLC** All rights reserved. **DMCA** NEW	
http://www.pubmedcentral.nih.gov/articlerender.fcgi?artid=1165278	Written by T Suzuki and E Takahashi Articles from Biochemical Journal are provided here courtesy of **The Biochemical Society**	Last Viewed: 6th October 2008
Images: http://www.bmrb.wisc.edu/metabolomics/standards/caffeine/lit/9684.png	Copyright © The Board of Regents of the University of Wisconsin System. Last Modified: Thursday, 15-Nov-2007 22:38:31 CST	Last Viewed: 6th October 2008
http://www.chemcool.com/regents/kineticsequilibrium/aim4.h9.jpg	Publisher not available	Last Viewed: 6th October 2008
http://www.rsc.org/ej/AN/2001/b104584a/b104584a-f1.gif	© Royal Society of Chemistry 2008	Last Viewed: 6th October 2008
http://www.steamytea.ie/acatalog/teatypes.gif	Copyright Steamy 07 - Established by Dermot and Tina	Last Viewed: 6th October 2008
http://www.webchem.net/images/kinetics/wpe1.jpg	Disclaimer: The content of this web site is provided for information purposes only. Every effort has been made to ensure that the content is reliable and accurate but no responsibility is accepted by the authors of the website for anything that is misleading or incorrect. Every effort has been made to trace the copyright holders of any material on this site, if we have overlooked anything, please contact us immediately. Last updated: 01 February 2005	Last Viewed: 6th October 2008

Books:

Chemistry For Advanced Level Third Edition	Written by Ted Lister and Janet Renshaw and published by Nelson Thornes	Last Viewed: 5th October 2008
IB Diploma Programme: Chemistry Course Companion	Written by Geoffrey Neuss and published by Oxford University Press	Last Viewed: 5th October 2008
IB Study Guides: Chemistry for the IB Diploma, Standard and Higher Level	Written by Geoffrey Neuss and published by Oxford University Press	Last Viewed: 5th October 2008

Other sources:

Caffeine extraction practical	Published by UWCSEA	Revised in June 2008	Last viewed: 19th September 2008
Caffeine extraction practical	Published by Bristol ChemLabS for National University of Singapore	Obtained in December 2007	Last viewed: 4th October 2008

Not a recognised way of setting out a bibliography. Books do not have year of publication.

RQ too broad. Theory very confused – probably too many dubious website consulted. Satisfactory only.

Appendix I

Variables –

Independent	The type of tea used – in terms of brand and manufacturer
Dependant	The moles of caffeine obtained
Controlled	The amount of reactants used in each trial – will be measured out accurately each time with appropriate error The mass of tea leaves used to stew tea and the length of time the tea is allowed to stew for – will be measured and time accurately with appropriate error What reactants are used, as some may be more effective than others – use the same ones throughout and do not vary the procedure in anyway -- For good measure, for every different brand and manufacturer, a minimum of three repeats will be done. Do the experiment two or three times beforehand to familiarise with the techniques to limit any error and to adjust the experiment where necessary.

Appendix II

Apparatus Used –

Beaker Number: 2 x 10 ml ± 2 4 x 250 ml ± 10
Glass stirring rod Number: 1
Conical flask Number: 4 x 250 ml
Suction filter funnel Number: 1 set
Separating funnel Number: 1 x 150 ml
Round-bottom flask Number: 1 x 50 ml
Petri dish Number: 18
Electric heating mantle and distillation set Number: 1 of each
(Pasteur) Pipette Number: 1 x 5 ml ± 0.05
Ice bath Number: 1 bucket filled with ice
Bunsen burner, heat proof mat, tripod, wire gauze and lighter Number: 1 of each
Filter paper Number: several sheets, approximately two per trial
Weighing scale Number: 1 with an error of ± 0.001 g
Clamp stand, boss and clamp Number: 3 x clamp stand 2 x boss 2 x clamp
Spatula Number: 3
Measuring cylinder Number: 2 x 10 ml ± 1 1 x 25 ml ± 0.5
Stopwatch Number: 1
Metal tongs Number: 1

Appendix III

Detailed Methodology –

1 *Making the tea solution*

1. Boil about 100ml of water in a 250 ml beaker, using a Bunsen burner (with tripod and wire gauze set up on a heat proof mat)
2. Weigh out 2g of tea leaves into another 250ml beaker.
3. Add 25 ml of boiling water to the tea leaves.
4. Leave for 5 minutes (using a stop watch to time) and stir three times with a glass stirring rod half way through.
5. Use the suction filter funnel to remove tea leaves, and pour the tea into a clean 250ml conical flask.
6. Weigh out 8g of sodium chloride into one 10ml beaker.
7. Add to the tea and heat the solution on the Bunsen until it starts to boil.
8. Weigh out 0.5g of calcium hydroxide into another 10ml beaker and add to the tea solution whilst still hot.
9. Gently place this into an ice bath and leave for about 5 minutes.
10. Once cool, use the suction filter to remove the solid impurities and pour the solution into a clean 250ml conical flask.

2 *Isolating the caffeine*

1. Use the solution from **1** to be poured into the separating funnel (set up, attached to the clamp stand with the boss and clamp).
2. Measure 8ml of propan-1-ol and pour into the separating funnel and place in stopper.
3. Upturn the mixture five times and leave to separate out.
4. Drain off the bottom layer into the original flask, and drain the propan-1-ol into a clean 250ml conical flask.
5. Repeat step 2. But use 5ml of propan-1-ol with the bottom layer from step 4.
6. Repeat step 3. and 4., however the propan-1-ol can be drained into the flask with the propan-1-ol from the first lot obtained in step 2.
7. Pour the propan-1-ol back into the separating funnel.
8. Measure out 13ml of the 2.5M sodium hydroxide.
9. Add this to the separating funnel and replace the stopper.
10. Upturn the mixture five times and leave to separate out.
11. Drain off the bottom layer into a 250ml conical flask (as a waster product) and drain the top layer into a clean 250ml conical flask.

3 *Purifying the caffeine*

1. Add two spatula's of anhydrous sodium sulphate to the top layer liquid from **2** .
2. Swirl and then leave until the liquid is clean and the sodium sulphate can be seen to be free flowing.
3. Set up the electric heating mantle (remembering to fasten it to a clamp stand for safety).
4. Set up for distillation.
5. Pour the clear liquid into a round-bottom flask, and heat with the electric heating mantle.

6. Distil until there is about 5ml of propan-1-ol left (it is useful to turn off the heating mantle before there is only 5ml left as the liquid is very hot and will continue to evaporate whilst waiting for it to cool).
7. Weigh a clean Petri dish (noting its initial mass).
8. Use a 5ml Pasteur pipette to remove exactly 5ml of propan-1-ol and dispense it into the Petri dish.
8. Leave overnight in a fume cupboard.
9. A solid should be seen, add 2ml of propanone to the Petri dish, swirling it, making sure that all the solid is covered.
10. Leave overnight in a fume cupboard.
11. Weigh the Petri dish (with a white crystalline solid, or caffeine, in it) and note its final mass.

Appendix IV

Safety Procedures –

<table>
<tr><th>Apparatus</th><th>Possible hazards</th><th>How to reduce the risks</th></tr>
<tr><td>Beakers, test tube, Petri dishes, Pasteur pipette, glass stirring rod, suction funnel, conical flask, round bottom flask, separating funnel</td><td>Glassware: may break. Also some is being heated so very hot and could burn</td><td>Take care using the equipment and if anything breaks: clear it up quickly. Also, if burnt, wash skin under cool water</td></tr>
<tr><td>Hot plate, kettle, boiling water</td><td>May burn or scald</td><td>Take care when using and wash skin under water if burnt or scalded</td></tr>
<tr><td>Bunsen burner</td><td>Open flame: may burn</td><td>Tie hair, wear goggles and take care. Wash skin under water if burnt</td></tr>
<tr><td>2.5M sodium hydroxide solution</td><td>Corrosive</td><td rowspan="6">Take care: wear goggles and tie hair. No flames near the propanone and propan-1-ol. Wear gloves when using the 2.5M sodium hydroxide solution. Caffeine should be kept in the fume cupboard and there should be limited handling.</td></tr>
<tr><td>Anhydrous sodium sulphate</td><td>Harmful</td></tr>
<tr><td>Propanone</td><td>Highly flammable, irritant to eyes</td></tr>
<tr><td>Propan-1-ol</td><td>Highly flammable, eye hazard</td></tr>
<tr><td>Calcium hydroxide</td><td>Eye hazard</td></tr>
<tr><td>PRODUCT: Caffeine</td><td>Can be fatal if inhaled, swallowed or absorbed through skin</td></tr>
</table>

Appendix V

Table of Raw Data for Ahmad™ teas –

		Initial mass of Petri dish / ± 0.001 g	Final mass of Petri dish / ± 0.001 g
Ceylon tea	Trial One	73.949	74.014
	Trial Two	28.512	29.200
	Trial Three	46.319	47.016
Darjeeling tea	Trial One	38.896	39.562
	Trial Two	39.505	40.126
	Trial Three	17.020	17.663
Earl Grey tea	Trial One	45.150	45.614
	Trial Two	43.321	43.742
	Trial Three	45.797	46.224

Table of Processed Data for Ahmad™ teas –

	***Mass of caffeine per two grams of tea* ± 0.002g**			***Average mass of caffeine in each tea per two grams* ± 0.002g**	***Average mass of caffeine per two grams* ± 0.2mg**	***Average mass of caffeine per gram* ± 0.001g**	***Average number of moles of caffeine per gram* ± 0.000005 moles**
	Trial one	**Trial two**	**Trial three**				
Ceylon tea	0.065	0.688	0.697	0.693	69.3	0.347	0.001789
Darjeeling tea	0.464	0.421	0.427	0.437	43.7	0.219	0.001129
Earl Grey tea	0.666	0.621	0.643	0.643	64.3	0.322	0.001660

****Anomaly – was disregarded during further calculations to find averages**

Appendix VI

Table of Raw Data for Dilmah™ teas –

		Initial mass of Petri dish / ± 0.001 g	Final mass of Petri dish / ± 0.001 g
Ceylon tea	Trial One	28.534	28.922
	Trial Two	38.007	38.196
	Trial Three	43.298	43.520
Darjeeling tea	Trial One	46.684	46.857
	Trial Two	29.204	29.396
	Trial Three	49.037	49.191
Earl Grey tea	Trial One	49.526	50.142
	Trial Two	41.381	42.018
	Trial Three	39.919	40.507

Table of Processed Data for Dilmah™ teas –

	***Mass of caffeine per two grams of tea* ± 0.002g**			***Average mass of caffeine in each tea per two grams* ± 0.002g**	***Average mass of caffeine per two grams* ± 0.2mg**	***Average mass of caffeine per gram* ± 0.001g**	***Average number of moles of caffeine per gram* ± 0.000005 moles**
	Trial one	**Trial two**	**Trial three**				
Ceylon tea	0.388	0.189	0.222	0.206	20.6	0.103	0.000531
Darjeeling tea	0.616	0.637	0.588	0.614	61.4	0.307	0.001582
Earl Grey tea	0.173	0.192	0.154	0.173	17.3	0.087	0.000448

****Anomaly – was disregarded during further calculations to find averages**

Appendix VII

Sample Calculation –

The following calculations use values from the Ceylon brand tea by the Ahmad™ manufacturer.

1) Final mass of Petri dish – initial mass of Petri dish
   = 74.014g – 73.949g
   = 0.065g ± 0.002

   Error = error in final mass + error in initial mass
   = ±(0.001g + 0.001g)
   = ±0.002g

2) Average mass of caffeine per two grams of tea in grams
   $= \frac{total\ mass\ of\ trials}{number\ of\ trials}$
   $= \frac{0.688g + 0.697g}{2}$
   = 0.693g ± 0.002
   the first value for Trial 1 that should have been included, was disregarded as it was too inaccurate

   Error $= \frac{total\ error\ of\ trials}{number\ of\ trials}$
   $= \pm\left(\frac{0.002g + 0.002g}{2}\right)$
   = ±0.002g

3) Average mass of caffeine per two grams of tea in milligrams
   = average mass in grams x 100
   = 0.693g x 100
   = 69.3mg ± 0.2

   Error = error in g x 100
   = ±(0.002g x 100)
   = ±0.2mg

4) Average mass of caffeine per gram in grams
   $= \frac{average\ mass\ of\ caffeine\ per\ two\ grams\ in\ grams}{2}$
   $= \frac{0.693g}{2}$
   = 0.347g ± 0.001

   Error $= \frac{error\ in\ average\ mass\ of\ caffeine\ per\ two\ grams\ in\ grams}{2}$
   $= \pm\left(\frac{0.002g}{2}\right)$
   = ±0.001g

5) Average moles of caffeine per gram of tea

$$= \frac{average\ mass\ of\ caffeine\ per\ gram}{molar\ mass\ of\ caffeine}$$

$$= \frac{0.347g}{(8 X 12) + (10 X 1) + (4 X 14) + (2 X 16)}$$

= 0.001789 moles ± 0.000005

Error = ±(percentage error in average mass of caffeine per gram x average moles of caffeine per gram of tea)

$$= \pm\left(\frac{0.001g}{0.347g} X 100\right) \text{ x } 0.001789 \text{ moles}$$

= ± 0.000005 moles

Assessment form (for examiner use only)

Candidate session number	0	0							

Assessment criteria

	Achievement level: First examiner	maximum	Second examiner
A research question	1	2	
B introduction	1	2	
C investigation	2	4	
D knowledge and understanding	2	4	
E reasoned argument	2	4	
F analysis and evaluation	2	4	
G use of subject language	2	4	
H conclusion	2	2	
I formal presentation	3	4	
J abstract	1	2	
K holistic judgment	2	4	
Total out of 36	20		

ame of first examiner: ______________________ Examiner number: ________
:APITAL letters)

ame of second examiner: ______________________ Examiner number: ________
:APITAL letters)