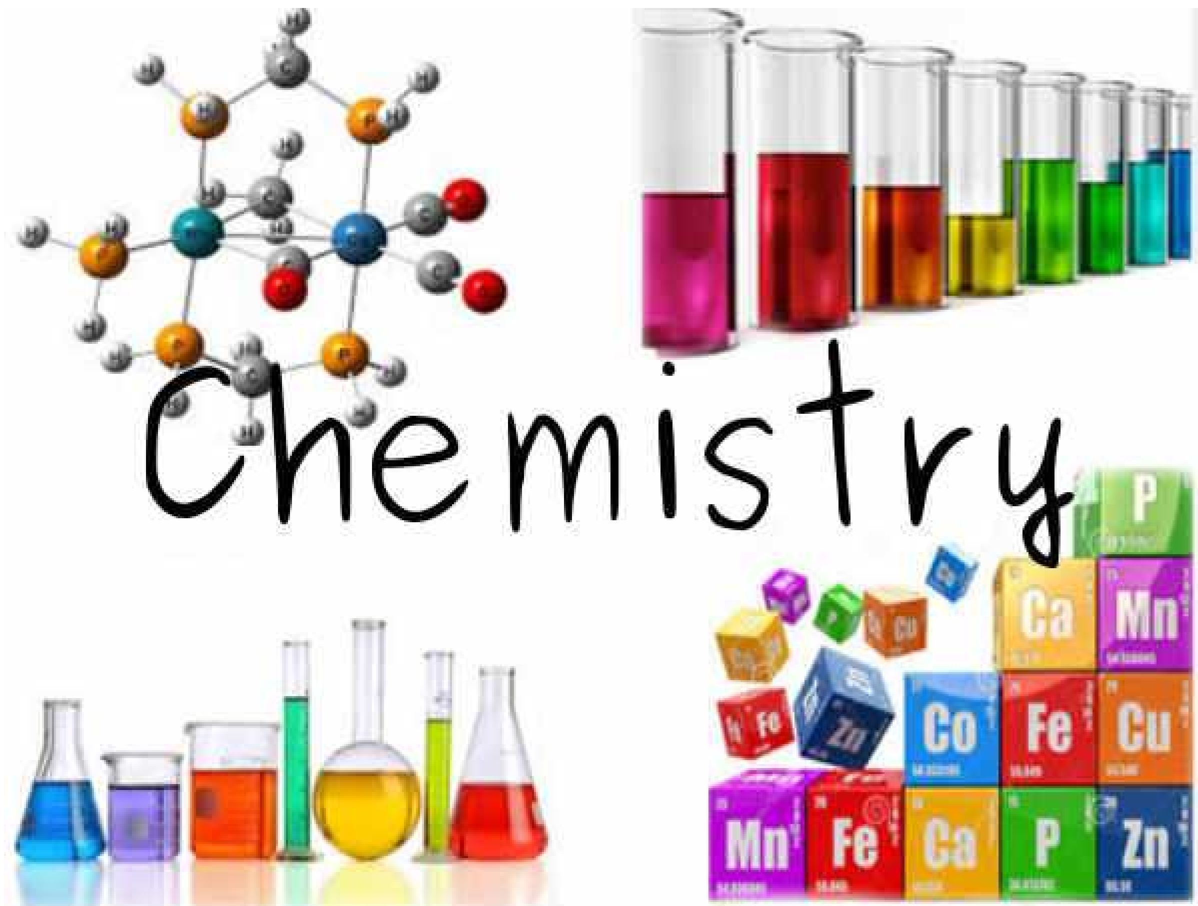
NAVRACHANA INTERNATIONAL SCHOOL VADODARA

IB DP CHEMISTRY

HIGHER LEVEL (HL)HANDBOOK

(Information in this document is resourced from IB subject guide and TSM)



Compiled by:

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SYLLABUS CONTENT

Core [95 hours]

- **Topic 1: Stoichiometric relationships**

1.1 Introduction to the particulate nature of matter and chemical change

1.2 The mole concept

1.3 Reacting masses and volumes

- **Topic 2: Atomic structure**

2.1 The nuclear atom

2.2 Electron configuration

- **Topic 3: Periodicity**

3.1 The periodic table

3.2 Periodic trends

- **Topic 4: Chemical bonding and structure**

4.1 Ionic bonding and structure

4.2 Covalent bonding

4.3 Covalent structures

4.4 Intermolecular forces

4.5 Metallic bonding

- **Topic 5: Energetics/thermochemistry**

5.1 Measuring enthalpy changes

5.2 Hess's law

5.3 Bond enthalpies

- **Topic 6: Chemical kinetics**

6.1 Collision theory and rates of reaction

- **Topic 7: Equilibrium**

7.1 Equilibrium

- **Topic 8: Acids and bases**

8.1 Theories of acids and bases

8.2 Properties of acids and bases

8.3 The pH scale

8.4 Strong and weak acids and bases

8.5 Acid deposition

- **Topic 9: Redox processes**

9.1 Oxidation and reduction

9.2 Electrochemical cells

- **Topic 10: Organic chemistry**

10.1 Fundamentals of organic chemistry

10.2 Functional group chemistry

- **Topic 11: Measurement and data processing**

11.1 Uncertainties and errors in measurement and results

11.2 Graphical techniques

11.3 Spectroscopic identification of organic compounds

Additional Higher Level (AHL) [60 hours]

- **Topic 12: Atomic structure**

12.1 Electrons in atoms

- **Topic 13: The periodic table – the transition metals**

13.1 First-row d-block elements

13.2 Coloured complexes

- **Topic 14: Chemical bonding and structures**

14.1 Covalent bonding and electron domain and molecular geometries

14.2 Hybridization

- **Topic 15: Energetics/thermochemistry**

15.1 Energy cycles

15.2 Entropy and spontaneity

- **Topic 16: Chemical kinetics**

16.1 Rate expression and reaction mechanism

16.2 Activation energy

- **Topic 17: Equilibrium**

17.1 The equilibrium law

- **Topic 18: Acids and bases**

18.1 Lewis acids and bases

18.2 Calculations involving acids and bases

18.3 pH curves

- **Topic 19: Redox processes**

19.1 Electrochemical cells

- **Topic 20: Organic chemistry**

20.1 Types of organic reactions

20.2 Synthetic routes

20.3 Stereoisomerism

- **Topic 21: Measurement and analysis**

21.1 Spectroscopic identification of organic compounds

Options [*15 hours – SL/ 25 hours – HL*]

- **A: Materials**

Core topics

A.1 Materials science introduction

A.2 Metals and inductively coupled plasma (ICP) spectroscopy

A.3 Catalysts

A.4 Liquid crystals

A.5 Polymers

A.6 Nanotechnology

A.7 Environmental impact – plastics

Additional higher level topics

A.8 Superconducting metals and X-ray crystallography

A.9 Condensation polymers

A.10 Environmental impact—heavy metals

- **B: Biochemistry**

Core topics

B.1 Introduction to biochemistry

B.2 Proteins and enzymes

B.3 Lipids

B.4 Carbohydrates

B.5 Vitamins

B.6 Biochemistry and the environment

Additional higher level topics

B.7 Proteins and enzymes

B.8 Nucleic acids

B.9 Biological pigments

B.10 Stereochemistry in biomolecules

- **C: Energy**

Core topics

C.1 Energy sources

C.2 Fossil fuels

C.3 Nuclear fusion and fission

C.4 Solar energy

C.5 Environmental impact—global warming

Additional higher level topics

C.6 Electrochemistry, rechargeable batteries and fuel cells

C.7 Nuclear fusion and nuclear fission

C.8 Photovoltaic and dye-sensitized solar cells

- **D: Medicinal chemistry**

Core topics

D.1 Pharmaceutical products and drug action

D.2 Aspirin and penicillin

D.3 Opiates

D.4 pH regulation of the stomach

D.5 Anti-viral medications

D.6 Environmental impact of some medications

Additional higher level topics

D.7 Taxol—a chiral auxiliary case study

D.8 Nuclear medicines

D.9 Drug detection and analysis

ASSESSMENT OUTLINE

HIGHER LEVEL ASSESSMENT SPECIFICATIONS

Component	Overall Weightage	Duration	Format & Syllabus Coverage
Paper 1	20	1 hr	40 multiple-choice questions on the core + AHL material.
Paper 2	36	2 ¼ hr	Data-based questions, short-answer questions and extended-response questions on the core and the AHL
Paper 3	24	1 ¼ hr	Questions on core and SL option material. Section A - short answer question on experimental work Section B - answer and extended-response questions from one option.
Externals Internals	80% 20% [Investigations + Group 4 project]		

PRACTICAL WORK AND INTERNAL ASSESSMENT

Internal Assessment Specifications 20%

INTERNAL ASSESSMENT CRITERIA

The new assessment model uses five criteria to assess the final report of the individual investigation with the following raw marks and weightings assigned.

Personal Engagement	Exploration	Analysis	Evaluation	Communication	Total
2(8%)	6(25%)	6(25%)	6(25%)	4(17%)	24(100%)

Students at SL are required to spend 40 hours, and students at HL 60 hours, on practical activities (excluding time spent writing up work). These times include 10 hours for the group 4 project and 10 hours for the internal assessment investigation. (Only 2–3 hours of investigative work can be carried out after the deadline for submitting work to the moderator and still be counted in the total number of hours for the practical scheme of work.)

RESOURCES:

- **Books:**

∝ Chemistry Course Companion, Sergey Bylikin, Gary Horner, Brian Murphy, David Tarcy, Oxford University Press.

∝ Pearson Baccalaureate Higher Level Chemistry 2nd edition, Catrin Brown, Mike Ford.

∝ IB Chemistry Study Guide: 2014 Edition: Oxford IB Diploma Program (Oxford IB Study Guides): Geoffrey Neuss.

Internal Assessment Group 4 Sciences
[Biology, Chemistry & Physics]

Weighting - 20% **Time – 10 hours**

The new assessment model uses five criteria to assess the final report of the individual investigation with the following raw marks and weightings assigned:

Personal Engagement:	**2**
Exploration:	**6**
Analysis:	**6**
Evaluation:	**6**
Communication:	**4**
TOTAL:	**24**

Personal engagement – 2 marks

This criterion assesses the extent to which the student engages with the exploration and makes it their own. Personal engagement may be recognized in different attributes and skills. These could include addressing personal interests or showing evidence of independent thinking, creativity or initiative in the designing, implementation or presentation of the investigation.

Mark	Descriptor
0	The student's report does not reach a standard described by the descriptors below.
1	The evidence of personal engagement with the exploration is limited with little independent thinking, initiative or creativity. The justification given for choosing the research question and/or the topic under investigation does not demonstrate personal significance, interest or curiosity. There is little evidence of personal input and initiative in the designing, implementation or presentation of the investigation.
2	The evidence of personal engagement with the exploration is clear with significant independent thinking, initiative or creativity. The justification given for choosing the research question and/or the topic under investigation demonstrates personal significance, interest or curiosity. There is evidence of personal input and initiative in the designing, implementation or presentation of the investigation.

Exploration – 6 marks

This criterion assesses the extent to which the student establishes the scientific context for the work, states a clear and focused research question and uses concepts and techniques appropriate to the Diploma Programme level. Where appropriate, this criterion also assesses awareness of safety, environmental, and ethical considerations.

Mark	Descriptor
0	The student's report does not reach a standard described by the descriptors below.
1–2	The topic of the investigation is identified and a research question of some relevance is stated but it is not focused. The background information provided for the investigation is superficial or of limited relevance and does not aid the understanding of the context of the investigation. The methodology of the investigation is only appropriate to address the research question to a very limited extent since it takes into consideration few of the significant factors that may influence the relevance, reliability and sufficiency of the collected data. The report shows evidence of limited awareness of the significant safety, ethical or environmental issues that are relevant to the methodology of the investigation.
3–4	The topic of the investigation is identified and a relevant but not fully focused research question is described. The background information provided for the investigation is mainly appropriate and relevant and aids the understanding of the context of the investigation. The methodology of the investigation is mainly appropriate to address the research question but has limitations since it takes into consideration only some of the significant factors that may influence the relevance, reliability and sufficiency of the collected data. The report shows evidence of some awareness of the significant safety, ethical or environmental issues that are relevant to the methodology of the investigation*.

5–6	The topic of the investigation is identified and a relevant and fully focused research question is clearly described. The background information provided for the investigation is entirely appropriate and relevant and enhances the understanding of the context of the investigation. The methodology of the investigation is highly appropriate to address the research question because it takes into consideration all, or nearly all, of the significant factors that may influence the relevance, reliability and sufficiency of the collected data. The report shows evidence of full awareness of the significant safety, ethical or environmental issues that are relevant to the methodology of the investigation.

Analysis – 6 marks

This criterion assesses the extent to which the student's report provides evidence that the student has selected, recorded, processed and interpreted the data in ways that are relevant to the research question and can support a conclusion.

Mark	Descriptor
0	The student's report does not reach a standard described by the descriptors below.
1–2	The report includes insufficient relevant raw data to support a valid conclusion to the research question. Some basic data processing is carried out but is either too inaccurate or too insufficient to lead to a valid conclusion. The report shows evidence of little consideration of the impact of measurement uncertainty on the analysis. The processed data is incorrectly or insufficiently interpreted so that the conclusion is invalid or very incomplete.

3–4	The report includes relevant but incomplete quantitative and qualitative raw data that could support a simple or partially valid conclusion to the research question. Appropriate and sufficient data processing is carried out that could lead to a broadly valid conclusion but there are significant inaccuracies and inconsistencies in the processing. The report shows evidence of some consideration of the impact of measurement uncertainty on the analysis. The processed data is interpreted so that a broadly valid but incomplete or limited conclusion to the research question can be deduced.
5–6	The report includes sufficient relevant quantitative and qualitative raw data that could support a detailed and valid conclusion to the research question. Appropriate and sufficient data processing is carried out with the accuracy required to enable a conclusion to the research question to be drawn that is fully consistent with the experimental data. The report shows evidence of full and appropriate consideration of the impact of measurement uncertainty on the analysis. The processed data is correctly interpreted so that a completely valid and detailed conclusion to the research question can be deduced.

Evaluation – 6 marks

This criterion assesses the extent to which the student's report provides evidence of evaluation of the investigation and the results with regard to the research question and the accepted scientific context.

Mark	Descriptor
0	The student's report does not reach a standard described by the descriptors below.
1–2	A conclusion is outlined which is not relevant to the research question or is not supported by the data presented. The conclusion makes superficial comparison to the accepted scientific context. Strengths and weaknesses of the investigation, such as limitations of the data and sources of error, are outlined but are restricted to an account of the practical or

	procedural issues faced. The student has outlined very few realistic and relevant suggestions for the improvement and extension of the investigation.
3–4	A conclusion is described which is relevant to the research question and supported by the data presented. A conclusion is described which makes some relevant comparison to the accepted scientific context. Strengths and weaknesses of the investigation, such as limitations of the data and sources of error, are described and provide evidence of some awareness of the methodological issues* involved in establishing the conclusion. The student has described some realistic and relevant suggestions for the improvement and extension of the investigation.
5–6	A detailed conclusion is described and justified which is entirely relevant to the research question and fully supported by the data presented. A conclusion is correctly described and justified through relevant comparison to the accepted scientific context. Strengths and weaknesses of the investigation, such as limitations of the data and sources of error, are discussed and provide evidence of a clear understanding of the methodological issues involved in establishing the conclusion. The student has discussed realistic and relevant suggestions for the improvement and extension of the investigation.

Communication– 4 marks

This criterion assesses whether the investigation is presented and reported in a way that supports effective communication of the focus, process and outcomes.

Mark	Descriptor
0	The student’s report does not reach a standard described by the descriptors

	below.
1–2	The presentation of the investigation is unclear, making it difficult to understand the focus, process and outcomes. The report is not well structured and is unclear: the necessary information on focus, process and outcomes is missing or is presented in an incoherent or disorganized way. The understanding of the focus, process and outcomes of the investigation is obscured by the presence of inappropriate or irrelevant information. There are many errors in the use of subject-specific terminology and conventions.
3–4	The presentation of the investigation is clear. Any errors do not hamper understanding of the focus, process and outcomes. The report is well structured and clear: the necessary information on focus, process and outcomes is present and presented in a coherent way. The report is relevant and concise thereby facilitating a ready understanding of the focus, process and outcomes of the investigation. The use of subject-specific terminology and conventions is appropriate and correct. Any errors do not hamper understanding.

CHEMISTRY INVESTIGATION

FACTORS EFFECTING THE BOILING AND MELTING POINTS IN ORGANIC HOMOLOGOUS SERIES.

Introduction

The idea for this investigation came about when we were learning about trends in physical properties in homologous series. With regards to alkanes we saw that the boiling point increases with increasing carbon number due to stronger van der Waal's forces as the temporary dipoles increase. However according to Brown and Ford[i] "the increase is not linear, but steeper near the beginning as the influence of increased chain length is proportionally greater for the small molecules".

EX: Going towards fulfilling "The background information provided for the investigation is entirely appropriate and relevant and enhances the understanding of the context of the investigation. "

Also I have seen that for compounds of similar molar masses (so that the strength of van der Waal's forces are similar) that the addition of functional groups into the hydrocarbon chain make a very great difference to the melting and boiling temperatures. For example the permanent dipole due to the carbonyl group in aldehydes and ketones results in a stronger dipole-dipole forces and so a higher boiling or melting point. The OH group in alcohols will cause an even higher boiling and melting temperature because it causes the strongest intermolecular force, hydrogen bonding to occur. This is supported if we take three compounds of similar molar mass, propane, ethanol and ethanol and compare their boiling temperature.

EX: More relevant background information.

	Mr (g mol^{-1})	Strongest intermolecular force	Boiling Temperature [ii] (°C)
Propane	44	Van der Waal's	-42
Ethanal	44	Dipole-Dipole	20
Ethanol	46	Hydrogen Bonding	78

From these values we see that the effect on the boiling temperature of adding a carbonyl or hydroxyl group is very large. But these are small molecules and I wondered if again the effect will be reduced with increasing hydrocarbon chain length because the proportionate effect of the functional group will get less and the aldehyde, ketone or alcohol will become more "alkane" in nature as the chain length increases. Will we see the melting and boiling points of the aldehydes, ketones and alcohols converge on those of the alkanes and if so at what chain length does the effect of a carbonyl or hydroxyl group become insignificant?

PE: Evidence of curiosity arising out of their classroom learning.

When looking at the effects of carbonyl or hydroxyl group one other possible influencing factor is the position on the chain of the carbonyl or hydroxyl group. I can imagine that a functional group hidden in the middle of a long hydrocarbon chain may not be able to approach and attract a close by molecule as easily as a functional group at the end of a chain. So my second aim is to see if a

PE: Independent thinking about the research question.

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functional group at the end of a chain will have a greater, lesser or the same effect on the intermolecular forces as one in the middle of a chain?

Research Questions

C: Very clearly presented and clarified research questions. Good.

(i) Will the melting and boiling points of the aldehydes, ketones and alcohols converge on those of the alkanes as we increase the carbon number and if so at what chain length does the effect of a carbonyl or hydroxyl group become insignificant?

(ii) What will be the effect on the melting and boiling points of changing the position of the functional group in the ketone of alcohol.

EX: The topic of the investigation is identified and a relevant and fully focused research question is clearly described.

Methodology

The dependent variables in this investigation are the melting and boiling points of the compounds in the homologous series: alkanes, aldehydes, 2-ketones, 3-ketones, 1-alcohols, 2-alcohols and 3-alcohols. The independent variables are the molar mass of the compound and the identity and position of the functional group

A control variable is that I will only look at compounds with linear hydrocarbon chains so there will be no added effect from branching.

When assessing the effect of the identity and position of the functional group I will be graphing the melting and boiling temperatures against the Molar Mass of the compound.

This investigation will use data available from two databases

1. CRC Handbook of Chemistry and Physics, 85th Edition, CRC Press, 2004
2. The RSC Chemspider online chemical database[iii]

EX: There are other databases available through the web but this was sufficient to address research question.

The Chemspider database contains experimental data and predicted data from ACD/LABS (boiling point only) and EPISuite. The predicted data was only to be used where an experimentally determined value was not available in the CRC Handbook or the Chemspider website.

The CRC Handbook was the first choice source of data since it is a resource that has been available for many years and I would assume many people have cross checked the data. Also once I was able to find a compound e.g. hexane, it was very quick and easy to read off values for hexanal, 1-hexanol, etc, since they were adjacent in the table of physical properties. In Chemspider I had to make a separate formula search for each one which was much slower.

EX: Good consideration regarding reliability of data.

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Raw Data

C: No use of compound names and a lot of empty cells do make the data tables a little hard to follow. However they bring together a large amount of data quite concisely (better than multiple tables for each homologous series) and there is a logic to their construction with the data organised according to ascending Mr.

DATA TABLE 1 Melting Pts		Melting Point (± 1 ºC)						
Number Carbons + Oxygens	Mr (±0.5 g/mol)	Linear Alkanes	Linear Aldehydes	Linear 2-ketones	Linear 3-ketones	Linear 1-alcohols	Linear 2-alcohols	Linear 3-alcohols
1	16	-182						
2	30	-183	-92					
2	32					-98		
3	44	-188	-123					
3	46					-114		
4	58	-138	-80	-95				
4	60					-124	-88	
5	72	-130	-97	-87				
5	74					-89	-89	
6	86	-95	-92	-77	-39			
6	88					-78	-73	-69
7	100	-91	-56	-56	-55			
7	102					-47	-51	-51
8	114	-57	-43	-35	-39			
8	116					-33	-39	-70
9	128	-53		-16				
9	130					-15	-32	-45
10	142	-30	-19	-8	-8			
10	144					-5	-35	22
11	156	-26	-4	14	1			
11	158					7	-1	-8
12	170	-10	-2	15	9			
12	172					16	0	
13	184	-5	12	21				
13	186					24	19	
14	198	6	14	31	31			
14	200					32	23	32
15	212	10	30	35	34			
15	214					38	34	32
16	226	18	25	20				
16	228					44	35	39
17	240	22	35		43			
17	242					49	44	50
18	254	28	36	48				
18	256					61	54	
19	268	32	46		51			
19	270					58		
20	282	36		57				
20	284					62		

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DATA TABLE 2 BOILING PTS		Boiling Point (± 1 ºC)						
Number Carbons + Oxygen	Mr (±0.5 g/mol)	Linear Alkanes	Linear Aldehydes	Linear 2-ketones	Linear 3-ketones	Linear 1-alcohols	Linear 2-alcohols	Linear 3-alcohols
1	16	-161						
2	30	-89	-19			65		
2	32					65		
3	44	-42	20					
3	46					78		
4	58	-1	48	56				
4	60					97	82	
5	72	36	75	80				
5	74					118	100	
6	86	69	103	102	102			
6	88					138	119	116
7	100	98	131	128	124			
7	102					158	140	135
8	114	126	153	151	147			
8	116					176	159	157
9	128	151	171	173	168			
9	130					195	179	171
10	142	174	191	195	190			
10	144					213	194	195
11	156	196	209	210	203			
11	158					231	211	213
12	170	216	**223**	232	227			
12	172					245	230	230
13	184	235	249	247	244			
13	186					260	252	247
14	198	254	**280**	263	**260**			
14	200					274	**265**	**261**
15	212	271	260	279	275			
15	214					287	284	276
16	226	287	285	294	289			
16	228					300	284	290
17	240	302	298	318	303			
17	242					312	314	304
18	254	316	310	320	316			
18	256					324	308	318
19	268	330	321	332	328			
19	270					335	319	331
20	282	343	332	344	340			
20	284					345	330	345

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Key to Data Sources in Data Tables

Blue font – CRC Handbook **Green Font – Chemspider Experimental**

Red Font = ACD/Labs prediction **Mustard Font – EPI Suite**

Uncertainty in Raw Data

The experimental data were cited with varying precision ranging from zero to three decimal places. Also the melting temperature was sometimes cited as a range. Where a range was given I have chosen the midpoint and have rounded off to the nearest integer value.

EX: Again described methodology regarding uncertainty of data. Good.

The data sources were evaluated by looking at some example compounds where experimentally determined data is available as well a prediction given

EX: Once again methodology is evaluating reliability of data. Good

Table 3: Evaluation of Data Sources

Compound	CRC Handbook Experimental data		Chemspider Experimental data		Chemspider ACD/Labs Predicted Data		Chemspider EPISuite Predicted Data	
	M.Pt (ºC)	B.Pt (ºC)	M.Pt (ºC)	B.Pt (ºC)	M.Pt (ºC)	B.Pt (ºC)	M.Pt (ºC)	B.Pt (ºC)
Hexane	-95	69	-95	69	NA	69	-94	72
Pentanal	-92	103	-92	103	NA	104	-68	109
1-Pentanol	-78	138	-79	137	NA	138	-50	137

Looking at Table 3 it is clear that there is usually good agreement between the CRC Handbook and Chemspider experimentally sources.

The ACD Labs predicted values for boiling temperatures appear quite close to experimental and can be used where experimental data is not available. At higher temperatures the experimental values in the CRC handbook relate to that measured at lower than atmospheric pressure. This could be because the boiling temperature at normal atmospheric pressure is very higher and the compounds may thermally decompose before the predicted boiling temperature.

The EPISuite predicted data is not so reliable. There is some variation in the boiling points and large variation in the melting temperature data. As a result I have omitted the EPI Suite data in the analysis section below.

A: Comments on lack of reliability of the EPI Suite data and understands the impact this will have on the validity of the results and so chooses to eliminate its data from analysis

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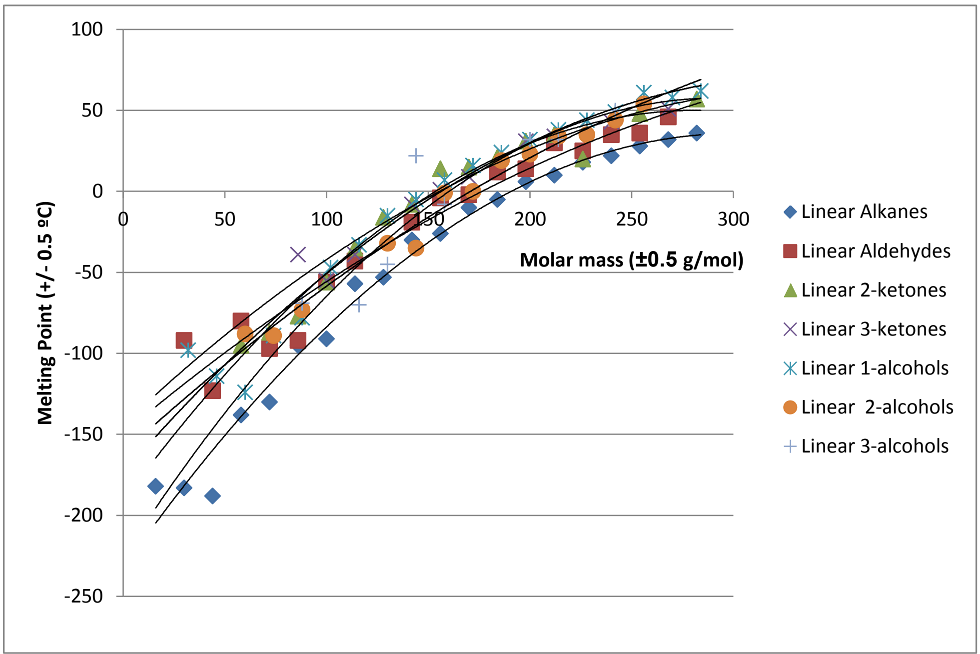
Analysis and Discussion

Part (i) Effect of chain length on the comparative melting and boiling points of the alkanes, aldehydes, ketones and alcohols.

The first two graphs below represent all the gathered data (except the discarded EPISuite predicted data).

Graph 1 – Melting points Plotted against Molar Mass for each Homologous Series

C: Trend lines are rather cramped in presentation making it hard to view individual trends, however it does enable a comparison to be seen. Graph is presented appropriately (scale, precision, units, uncertainties.)
A: Appropriate best fit line and correctly plotted points.



Graph 1 (the melting temperatures) showed a trend but it is not very well defined. The trend-lines of the different homologous series do not converge as clearly as with the boiling temperatures below. This is not something that I was expecting at first and I cannot easily explain the fact that melting temperatures of aldehydes, ketones and alcohols remain significantly above the melting temperature of the alkane of similar molar mass. From the data sources the melting temperatures were not so well defined as boiling temperatures and were often given as a range of temperatures. This could be an area for further study.

A. Graph clearly represents data but importantly the student has not over interpreted the graph. There is not a clear convergence and the student has not unduly claimed so which is quite insightful.

EV: Recognizing impact of uncertainty on the possible conclusion.

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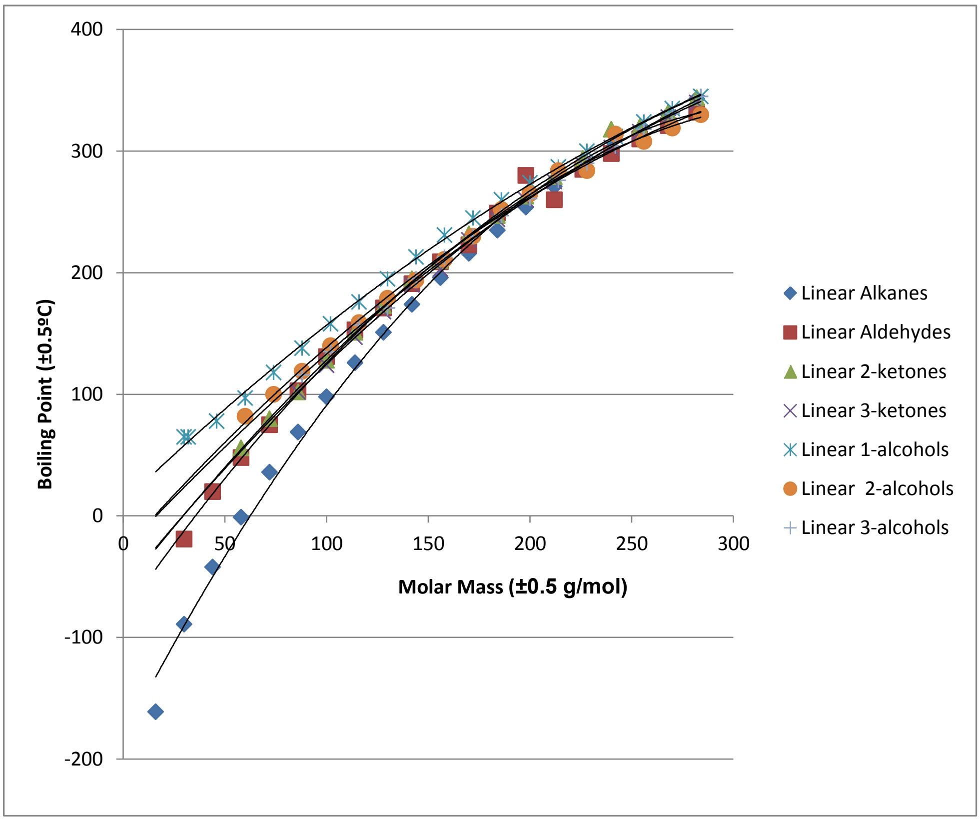
Graph 2 – Boiling points Plotted against Molar Mass for each Homologous Series



C: Again trend lines are rather cramped in presentation making it hard to view point of convergence. Graph 3 with just the experimental data reveals this more clearly. Graph is presented appropriately (scale, precision, units, uncertainties.)

From Graph 2 we see that the boiling temperatures are well defined and the smooth trend-lines do indicate the boiling temperature values for the alkanes, aldehydes, ketones and alcohols do appear to converge at molar mass values above 220 $gmole^{-1}$. This is not surprising since the influence on the intermolecular forces of the carbonyl and hydroxyl groups reduces as the hydrocarbon chain increases and dominates the character of the molecule.

A: Graph allows for valid interpretation.

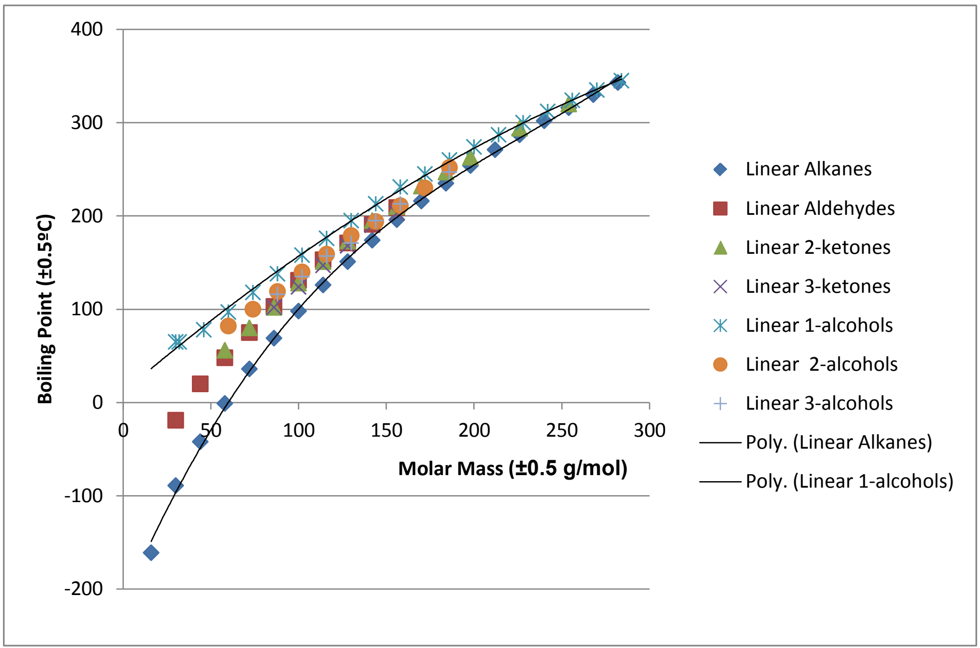
C: Use of correct convention for representing unit. Should be 220 $gmol^{-1}$, but not sufficient to hamper understanding.

EV: Student has described AND justified a valid conclusion.

If we look only at the CRC Handbook experimental data and not use any predicted data then the convergence is even more clear (and removes the anomalous linear aldehyde data points at 198 and 212 $gmol^{-1}$) as shown in Graph 3 below.

A: This was an excellent step to remove the predicted data. Fine reflective thinking while processing.

Graph 3: CRC Handbook Experimental Data Only



Graphs 2 and 3 also show that at low molar masses that the trend in boiling points is

alcohols > aldehydes/ketones > alkanes

which agrees with hydrogen bonding being stronger than dipole-dipole forces which are stronger than van der Waal's forces. At higher molar masses the difference gets much less.

EV: Again justifying the conclusion.

Part(ii). Effect on the boiling points of the functional group position in the aldehyde/ketones and alcohols.

Because the boiling points are so much clearer than the melting points the rest of my analysis will be based only on the boiling points.

A: A sensible decision.

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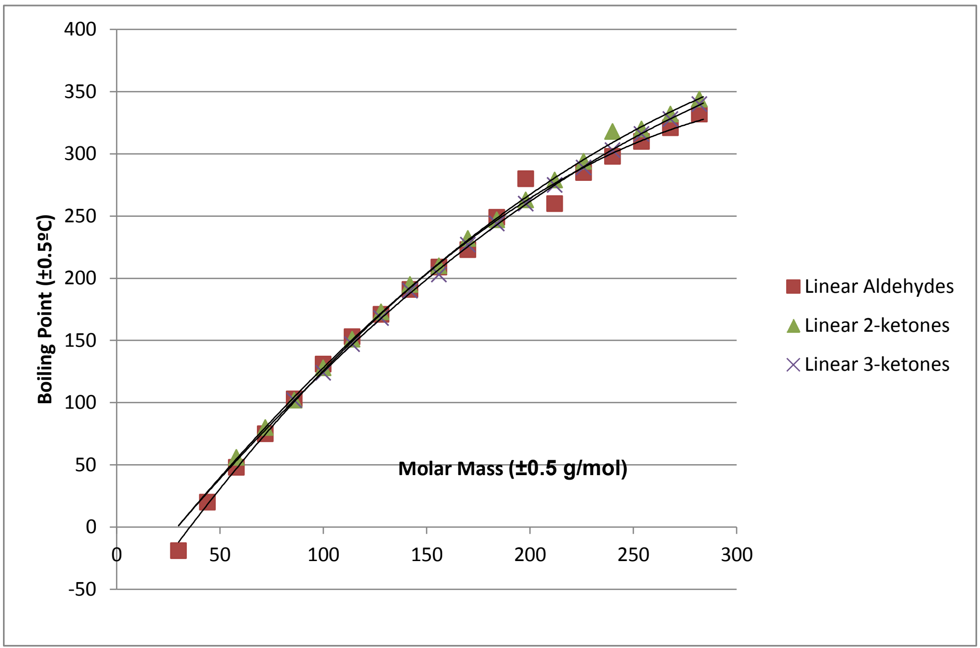
Graph 3 Effect on the Boiling Points of the carbonyl position in the aldehyde and ketones



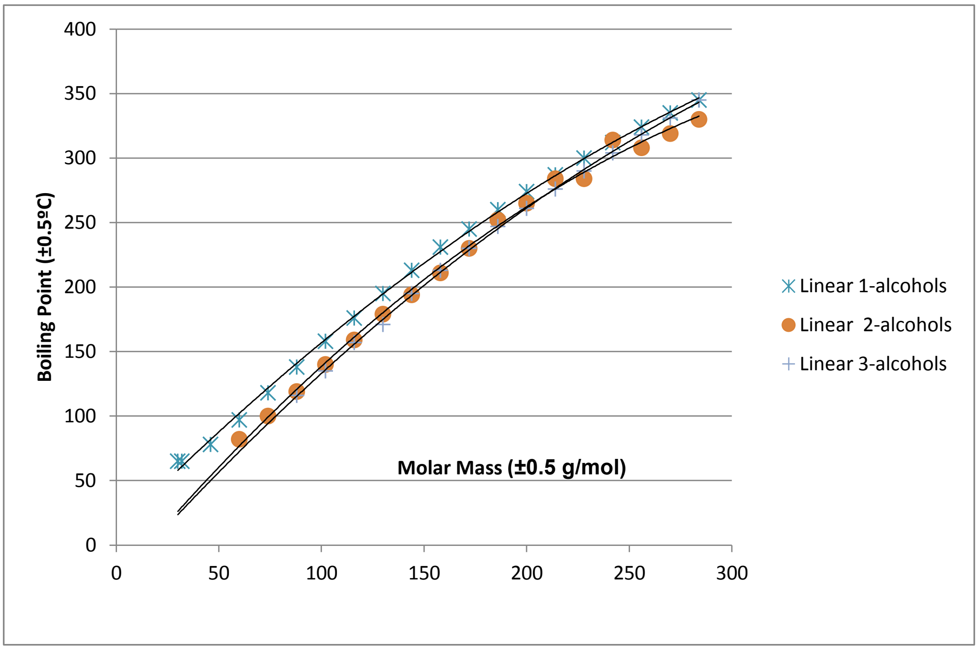
There is very little difference in the melting points between the aldehyde, 1-ketone and 2-ketone isomers at each molar mass and the graph lines are very similar. There is a strange anomaly with the data for the aldehydes $C_{13}H_{18}O$ and $C_{14}H_{30}O$ where the respective boiling points of 280°C and 260ºC seem to be swapped around. I have checked again the experimental data on ChemSpider and those are the values given. The values are not available in the CRC Handbook to double check and this means that I am not very confident in their correctness.

EV: Clear evidence of appreciating limitations in data and understanding methodological implications.

If the data in the table is looked at in Data table 2 we can see that where experimental values are are available the 3-ketone has a slightly lower boiling point by between 1 and 6 °C. But the predicted values are often higher than the corresponding aldehyde and 2-ketone. I suggest that 3 ketones have a lower melting point than the aldehydes and 2-ketones but the effect is not large enough to state confidently.

EV: Once again student gets it right by not overstating their interpretation.

Graph 4 Effect on the Boiling Points of the OH group position in the alcohols



Graph 4 shows that the boiling points of the 1-alcohols are significantly higher than the corresponding 2-alcohols and 3-alcohols. Where we have the CRC Handbook experimental data available for all three series (up until the dodecanol $C_{12}H_{26}O$ isomers) the 2- and 3- alcohols have similar boiling temps which are significantly below the 1-alcohols. I can make the hypothesis that this is because the OH group at the end of the chain in the 1-alcohols can more easily approach from a variety of angles another OH group from another 1-alcohol molecule. If the OH group is in the middle of a chain (like a 3-alcohol) then there are less ways that two molecules can align and attract each other. I have shown these possibilities in Figure 1 and 2 below with Chemsketch 3D images of 1-hexanol and 3-hexanol. It can be seen that there are more possible orientations where the 1-hexanol molecule OH groups can approach and H-bond

EV: Clear conclusion supported by the data is given. The student then goes on to try to justify within a relevant scientific context.

PE: This personal hypothesis shows some real original thinking. Shame that the student hasn't found any literature support for the hypothesis. That would then have been close to perfect! As it is this is an outstanding effort.

Figure 1: 1-Hexanol

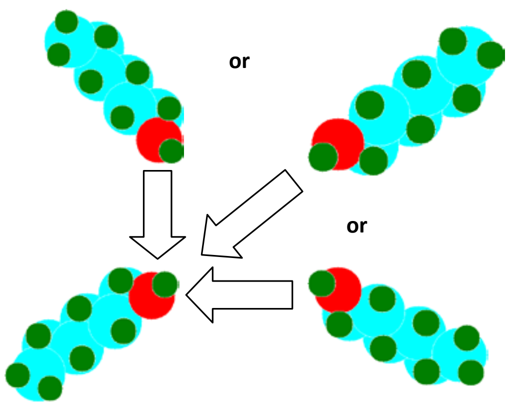


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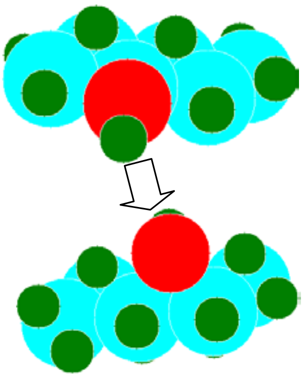
Figure 2. 3-Hexanol



Conclusion

The main conclusions to this research are the answers to the two parts of the research question given earlier

(i) The boiling points of the aldehydes, ketones and alcohols do converge on those of the alkanes as we increase the carbon number and above 200gmol^{-1} the differences become minimal. The melting points were less well defined and although there is some convergence it is not so clear as for the boiling points

(ii) The effect of boiling point on changing the position of the functional group in the alcohol is significant. 1-alcohols with the OH group at the end of the chain have a higher boiling temperature than the 2- and 3-alcohols.

C: Clearly restated main conclusions.

There were other interesting findings such as the significant differences in how well defined the melting and boiling temperatures were and the fact that some predicted values available in the web-based databases were very unreliable. These can be the basis for further study.

EV: Not very strong suggestions and no real suggestions for modifications.

[i] C. Brown and M. Ford, Higher Level Chemistry, p 367, Pearson Baccalaureate, 2009
[ii] CRC Handbook of Chemistry and Physics, 85th Edition, CRC Press, 2004
[iii] http://www.chemspider.com, last accessed on 11/3/2012

AN INVESTIGATION INTO THE DEPENDENCE OF EGG PROTEIN DENATURATION ON TEMPERATURE.

Aim

The aim of this investigation was to investigate how the rate of denaturation of egg white proteins is dependent on temperature and to experimentally determine the Activation Energy of the denaturation process.

EX- Research questions are clearly stated and the purpose is well focused.

Introduction.

The original idea for this project came from a lesson on boiling temperature and vapour pressure when we learned why it takes longer for an egg to hard boil at high altitude (due to the lower boiling temperature of water). This topic stimulated many thoughts. How is the time it takes to boil an egg dependant on temperature? Can the time taken to exactly hard boil an egg be predicted over all temperatures? Below what temperature do eggs cease to hard boil?

PE- The student clearly describes the whole process that resulted in his/her engagement in this investigation.

I decided that the investigation would concentrate on determining one important parameter which is the Activation Energy barrier to egg protein denaturation. If this can be determined then predictions of the egg's behaviour during boiling at a range of temperatures can be made and then tested.

EX- The choice of research is well explained.

Background

This project has two main theoretical bases, the principles of kinetics and process of the nature of protein denaturation, which I will describe below.

Part A: Kinetics and the Arrhenius Equation

The way temperature affects the rate of a reaction is explained by the Figure 1 below[1].

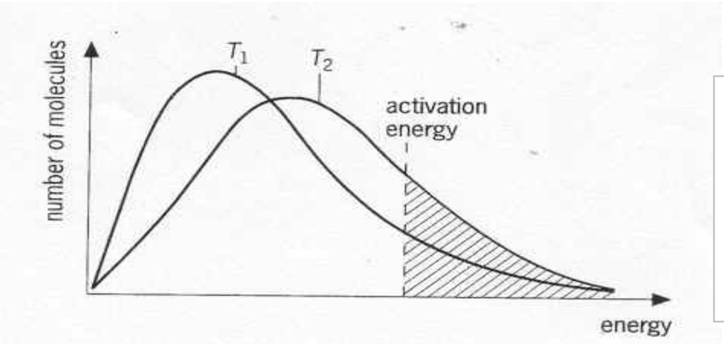


Figure 1 [1]: Maxwell-Boltzman graph where $T_2 > T_1$.

1

Only collisions with more energy than that of Activation Energy (the minimum energy that must be surpassed in order for a chemical reaction to take place) will cause a reaction. Therefore, in the graph above, the shaded area represents those collisions.

According to theory, as temperature increases, the molecule velocities increase, and therefore, both the frequency of collision between molecules is greater and a greater proportion of collisions cause a reaction. In figure 1, this is apparent. At the lower temperature, $T_{1,}$ the fraction of molecules reacting is less than of T_2 (shaded area on graph). The rate of reaction is proportional to the number of molecules with more energy than Ea and increases exponentially with temperature.

The relationship between reaction rate and temperature is expressed by the **Arrhenius equation** which relates the rate constant of a reaction k to the absolute temperature T:

$$k = Ae^{-(Ea/R.T)}$$

where k= rate constant, Ea= Activation energy, T= Reaction Temperature, R= Gas constant and A = Arrhenius constant which is a factor that relates to the orientation of collision; only molecules colliding in the correct orientation with sufficient energy react.

Note that the Arrhenius equation is an exponential function and only applies when the activation energy lies within the exponential decay part of the curve to the right hand side of the Boltzman distribution graph in Figure 1.

EX- The student provides a good support for the chosen approach.

EX- The student establishes the scientific context for the investigation through a discussion on its significance.

Part B: Proteins & Denaturation

Proteins are formed by a combination of amino acids containing often 50 to 1000 amino acid residues). All proteins, independent of their nature (shape, complexity etc…) have structures, which are divided into four categories: primary, secondary, tertiary and quaternary.

The primary structure is mainly concerned with protein polypeptide chains (subunits) and with its amino acid sequence. In the secondary structure, there are different types of energetically stable three-dimensional structures of the polypeptide chain (also referred to as conformations). For some proteins, their polypeptide chain might form a β-pleated sheet and for others it might follow the spiral a-helix conformation. The tertiary structure is the overall three-dimensional appearance of the protein which is held together by strong intermolecular forces (e.g. Hydrogen bonding). For example, a globular protein such as in egg white, is approximately spherical and folding is extensive to obtain a compact tertiary structure. Lastly, the interaction of various polypeptide chains in a non-covalent way to pattern the protein molecule is said to present the quaternary structure.

Denaturation is when the biological activity of a protein is lost and disruption in the secondary, tertiary and quaternary structure of a protein occurs due to changes in temperature, pH, ionic strength, or due to an addition of organic solvents. For instance, when egg white is exposed to heat, it thickens and changes color. At that point, denaturation has occurred and all its structure has been disrupted, except for its primary structure, and an alternative energetically stable three dimensional structure is formed. It is the energy barrier to this process of permanently disrupting the three dimensional structure of the egg protein that is the focus of this investigation.

EX- Relevant scientific concepts are correctly considered.

Methodology

EX- The methodology allows the use of concepts and techniques appropriate to Diploma level.

A common procedure (Hill, G & Holman, J (2001))[2] to determining the Ea, is by measuring the time of reaction (in this case of final time of denaturation of egg proteins determined as the time when the film of egg white between the two microscope slides became opaque) at various different reaction temperatures using the Arrhenius equation:

C- The methodology could be easily repeated by others.

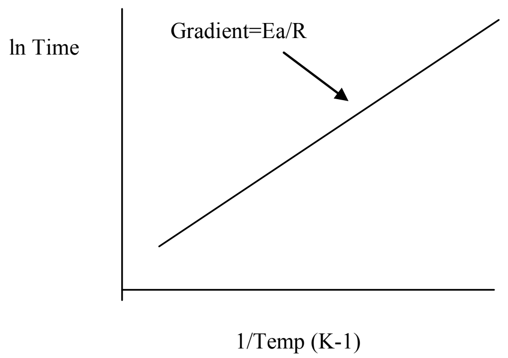
$$k = Ae^{-(Ea/R.T)} \Rightarrow \ln k = \ln A^{-(Ea/R.T)}$$

and since k is proportional to 1/Time:

$$\ln k = -\ln Time + a\ constant \rightarrow \ln Time = (Ea/R.T) - \ln A + a\ constant$$

Now, we can plot a graph, InTime versus 1/Temperature (in Kelvin) and calculate the gradient. Since we recognize the gas constant(R=8.3145 JK-1mol-1), we can determine the Activation energy:

Gradient = Ea/R → Ea = R x Gradient



3

EXPERIMENTAL PROCEDURE

The focus of the experimental work was to measure how long it took egg white and egg yolk to denature over a range of temperatures. The development of a suitable procedure was far more time consuming than originally anticipated since it proved difficult to experimentally determine exactly when the egg sample had 'boiled' (denatured). In the end some procedures yielded results and these experiments are described below. The final successful experiments only focused on the egg whites.

EX- There is a consideration of limitations in the methodology.

PE- The student presents a brief discussion on the development of the method including obstacles found during this process. This shows personal input and initiative.

The procedure was as below:

1. The egg white was separated from the egg yolk in a small beaker and a 500ml beaker was filled with tap water to heat over a flame.
2. With a syringe, a drop of egg white was put on the center of a preweighed microscope glass slide and then using another clean preweighed microscope glass slide, I pressed them together (with egg white in between) and wiped up the sides of the slides. They were weighed again.
3. Afterwards, the diameter of the circular shaped liquid egg white pressed between the two slides was measured.
4. Then, at different temperatures of the heated water slides were added to the water and were closely observed, as the stopwatch was running.
5. When I noticed denature of the egg white, I stopped the stopwatch and simultaneously placed the two slides in room temperature water to cool down.
6. In each experiment, recorded was the time the egg white took to denature and temperature it was at.

EX- The methodology allows the collection of data that are both sufficient and relevant.

EX- The methodology employed has taken most relevant variables into account.

4

Results

Egg white results

Diameter (+/- 0.1 cm)	Mass of egg white (+/- 0.005 g)	Temperature of water (+/- 0.5 °C)	Time of denaturation (+/- 0.5 sec)
2.5 by 5.0	0.01	25.0	Never denatured
2.5 by 5.0	0.01	30.0	Never denatured
2.5 by 4.5	0.01	35.0	Never denatured. Not even after 15 min.
2.5 by 5.0	0.01	40.0	Never denatured. Not even after 10 min.
2.5 by 5.0	0.02	45.0	Never denatured. Not even after 5 min.
2.5 by 5.0	0.01	50.0	Never denatured. Not even after 5 min.
2.5 by 5.5	0.01	55.0	Never denatured. Not even after 5 min.
2.5 by 5.0	0.01	60.0	Never denatured. Not even after 5 min.
2.5 by 5.0	0.01	62.5	49.9 sec.
2.5 by 5.0	0.01	62.5	49.7 sec.
2.5 by 5.0	0.01	65.0	32.8 sec.
2.5 by 4.5	0.01	67.5	21.0 sec.
2.5 by 5.5	0.01	70.0	15.9 sec.
2.5 by 5.5	0.01	75.0	11.0 sec.
2.5 by 5.0	0.01	80.0	8.0 sec.
2.5 by 5.0	0.01	81.0	7.6 sec.
2.5 by 5.0	0.01	82.5	7.0 sec.
2.5 by 5.0	0.01	84.0	6.4 sec.
2.5 by 5.0	0.01	85.0	6.0 sec.
2.5 by 5.0	0.01	86.0	5.5 sec.
2.5 by 5.5	0.01	87.5	4.9 sec.
2.5 by 5.0	0.01	89.0	4.2 sec.
2.5 by 5.0	0.02	90.0	4.0 sec.
2.5 by 5.0	0.01	91.0	3.8 sec.
2.5 by 5.5	0.02	92.5	3.5 sec.
2.5 by 5.0	0.01	94.0	3.3 sec.
2.5 by 5.5	0.01	95.0	3.0 sec.
2.5 by 5.0	0.01	97.5	2.4 sec.
2.5 by 5.0	0.01	97.5	2.5 sec.
2.5 by 5.0	0.01	100.0	2.1 sec.
2.5 by 5.0	0.01	100.0	2.2 sec.

A- Sufficient quantitative data has been collected. Uncertainties have been recorded although those for time are not consistent with the cited precision of the data.

5

ANALYSIS

C- The processing is easy to follow.

In order to find the activation energy I need to calculate ln Time and 1/Temperature values for the reaction temperatures where denaturation occurred

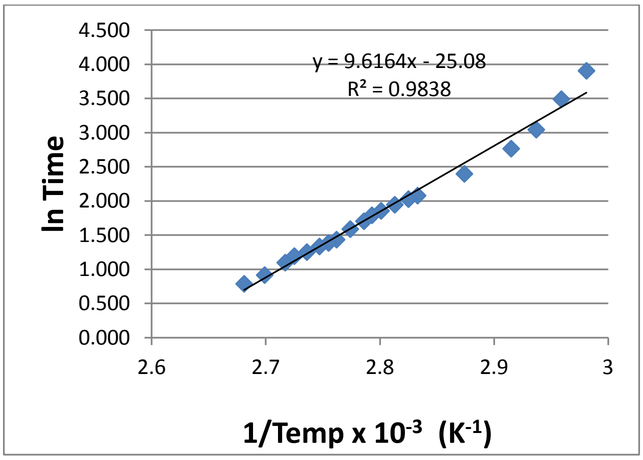
C- Tables are presented unambiguously.

Temperature(k)	Time(sec.)	ln Time	1/ Temp.(k^{-1})
298.0	-----	-----	
303.0	-----	-----	
308.0	-----	-----	
313.0	-----	-----	
318.0	-----	-----	
323.0	-----	-----	
328.0	-----	-----	
333.0	-----	-----	
335.5	49.7	3.906	$2.981x10^{-3}$
338.0	32.8	3.490	$2.959x10^{-3}$
340.5	21.0	3.045	$2.937x10^{-3}$
343.0	15.9	2.766	$2.915x10^{-3}$
348.0	11.0	2.398	$2.874x10^{-3}$
353.0	8.0	2.079	$2.833x10^{-3}$
354.0	7.6	2.028	$2.825x10^{-3}$
355.5	7.0	1.946	$2.813x10^{-3}$
357.0	6.4	1.856	$2.801x10^{-3}$
358.0	6.0	1.792	$2.793x10^{-3}$
359.0	5.5	1.705	$2.786x10^{-3}$
360.5	4.9	1.580	$2.774x10^{-3}$
362.0	4.2	1.435	$2.762x10^{-3}$
363.0	4.0	1.386	$2.755x10^{-3}$
364.0	3.8	1.335	$2.747x10^{-3}$
365.5	3.5	1.253	$2.736x10^{-3}$
367.0	3.3	1.194	$2.725x10^{-3}$
368.0	3.0	1.099	$2.717x10^{-3}$
370.5	2.5	0.916	$2.699x10^{-3}$
373.0	2.2	0.788	$2.681x10^{-3}$

C- Appreciation of decimal places evidenced in this table.

Graph 1. Plot of ln Time against 1/Temperature

C- Graphs are presented unambiguously.



Calculation to determine Activation energy, Ea.

Gradient from Excel derived linear equation

$= 9.6164 \times 10^3 = 9616$

Gradient= Ea/R so Ea= 9616x 8.314

Ea= 79974 J mol^{-1}

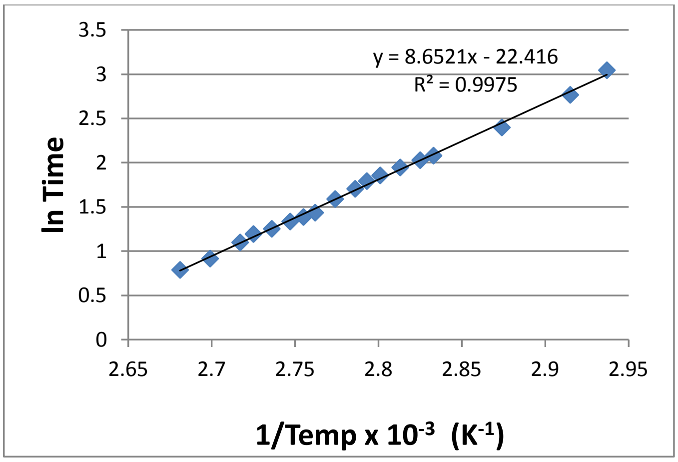
Ea = 80kJ mol^{-1}

The two data points corresponding to the lowest reaction temperatures at 335.5 and 338.0 K do not appear to conform to the linear plot. I have removed these two points as anomalous in the graph below and recalculated Ea.

EV--The student takes reliability into account.

A- Processing pays due consideration to anomalies.

Graph 2. Plot of ln Time against 1/Temperature with discarded data points



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Gradient from Excel derived linear equation

$= 8.6521 \times 10^3 = 8652$

Gradient= Ea/R so Ea= 8652x 8.314

Ea= 71932.73 J mol^{-1}

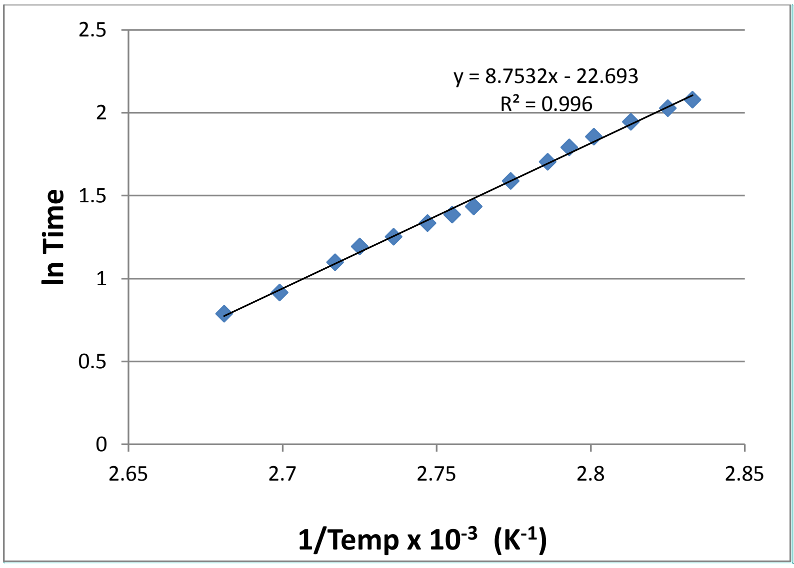
Ea = 72kJ mol^{-1}

A- Processing correctly uses chemical concepts and graphical analysis to determine Ea.

By cutting the data back further to a maximum 1/Temp value of 2.766×10^{-3} which represents the closely spaced data points the graph becomes

A- The student shows evidence of a good understanding of graphical analysis.

Graph 3. Plot of ln Time against 1/Temperature with further discarded data points



EV- Evidence supporting the student has considered the impact of uncertainties on results (line of best fit).

and Ea= 8753x 8.314

Ea= 72772.44 J mol^{-1}

Ea = 73kJ mol^{-1}

C- Correct use of significant figures.

The calculated Es results are tabulated below along with the R^2 correlation value that relates to how good the linear fit was in the graphs (with 1 being perfect fit)

A- The processing involves correctly constructed lines of best fit and makes use of R^2 for evaluating uncertainties.

	Graph 1	Graph 2	Graph 3
Ea (kJ mol^{-1})	80	72	73
R^2	0.9838	0.9975	0.996

EV- Evidence that the student understands the impact of uncertainties on results.

The best value is from graph 2 and the value from Graph 3 gives some idea as to the amount of uncertainty arising from the plots.

A- The processing presents a valid comparison which duly considers uncertainties and shows a good grasp of graphical analysis.

My final experimental value for Ea of egg protein denaturation = 72 ± 1 kJ mol^{-1}

A- Uncertainties considered in final value.

8

Conclusion and Evaluation

The initial aims of the investigation have been met. It has be seen that denaturation did not take place at 60°C and below. Above this temperature the rate of protein denaturation increases rapidly with temperature.

I was able to calculate an Activation Energy for the activation energy of egg protein denaturation and it was

Ea = 72 ± 1 kJ mol^{-1}

I could not find an exact **literature value** for the Ea of egg protein (albumin). One article[3] studied the effect at acidic pH's (which will change the Ea because acidic pH also denatures proteins) and gave the values as 36.7 and 50.0 kcal./mole which correspond to **150-200 kJ mol^{-1}**

My value is about a half or a third of this literature value. When I reflect on the simplicity of the method I am impressed that this investigation has arrived at a value that is so sensible in size.

It is also significant that the Arrhenius equation seems appropriate for the determination of egg protein denaturation as long as the temperature range for the measurements is kept within specifically defined limits. This is because the Arrhenius equation strictly applies to ideal gas reactions only although it has been widely used in the study of liquids and solution reactions where collision theory still holds and only the Arrhenius constant A is affected by the change of state.

However the denaturation reaction of proteins is not a collision reaction (it depends on the protein chains rotating and intermolecular forces breaking and reforming) and the theoretical basis of the equation no longer so obviously holds. There is no obvious reason why the plot of ln(Time) v 1/Temperature should have been so clearly linear. It is maybe the most interesting finding of this investigation that the relationship in the Arrhenius Equation still seems appropriate.

C- The report has been easy to follow, concise and shows a logical sequence.

C- Subject specific terminology is correctly used throughout the report.

C- The report makes use of subject-specific notation.

A- Comparison with scientific literature made.

EV- There are no clear suggestions of feasible extensions to this investigation.

EV- There are no clear suggestions on relevant and feasible alternatives to improve methodology.

EV- The reflections demonstrate a clear understanding of implications of the conclusion.

EV- Student considers limitations of the methodology.

9

References

1. http://www.webchem.net/notes/how_far/kinetics/rate_factors.htm, last accessed 3rd March 2012

2. Hill, G & Holman, J (2001). *Chemistry in Context: Laboratory Manual and Study Guide*, 5th Edition, pp 54-55, Surrey, Nelson

3. Investigations on proteins and polymers. VII. The denaturation of egg albumin, Robert J. Gibbs, M. Bier, F.F. Nord, Archives of Biochemistry and Biophysics, Volume 35, Issue 1, January 1952, Pages 216–228, Last accessed at http://www.sciencedirect.com/science/article/pii/S0003986152800670 on 4th March 2012

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4. http://chemistry.about.com/od/biochemistry/a/proteinstructur.htm, last accessed 26th February 2012

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