Use of Journal Articles as Assessment Resources in Chemistry

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It's the Keele difference.

Subject Benchmark Statement: Chemistry

QAA

https://www.qaa.ac.uk/quality-code/subject-benchmark-statements

4 Subject knowledge and understanding

4.1 Each higher education provider awarding qualifications in chemistry defines the content, nature and organisation of its programmes and modules. Consequently chemistry programmes offered by individual higher education providers will have their own particular characteristics.

4.2 Bachelor's degrees with honours programmes ensure that students:

- are fully conversant with major aspects of chemical terminology
- demonstrate a systematic understanding of fundamental physicochemical principles with the ability to apply that knowledge to the solution of theoretical and practical problems
- gain knowledge of a range of inorganic and organic materials
- demonstrate, with supporting evidence, their understanding of synthesis, including related isolation, purification and characterisation techniques
- demonstrate an understanding of the qualitative and quantitative aspects of chemical metrology and the importance of traceability
- develop an awareness of issues within chemistry that overlap with other related subjects
- develop knowledge and understanding of ethics, societal responsibilities, environmental impact and sustainability, in the context of chemistry
- develop an understanding of safe working practice, in terms of managing chemical toxicity, chemical stability and chemical reactivity, through knowledge-based risk assessments
- read and engage with scientific literature.

Subject Benchmark Statement: Chemistry

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Professional skills

5.7 In bachelor's degree with honours programmes, students develop:

- communication skills, covering both written and oral communication with a variety of audiences
- skills in the employment of common conventions and standards in scientific writing, data presentation, and referencing literature
- problem-solving skills, relating to qualitative and quantitative information
- numeracy and mathematical skills, including handling data, algebra, functions, trigonometry, calculus, vectors and complex numbers, alongside error analysis, order-of-magnitude estimations, systematic use of scientific units and different types of data presentation
- information location and retrieval skills, in relation to primary and secondary information sources, and the ability to assess the quality of information accessed
- information technology skills which support the location, management, processing, analysis and presentation of scientific information
- basic interpersonal skills, relating to the ability to interact with other people and to engage in teamworking
- time management and organisational skills, as evidenced by the ability to plan and implement efficient and effective ways of working
- skills needed to undertake appropriate further training of a professional nature
- other relevant professional skills such as business awareness.

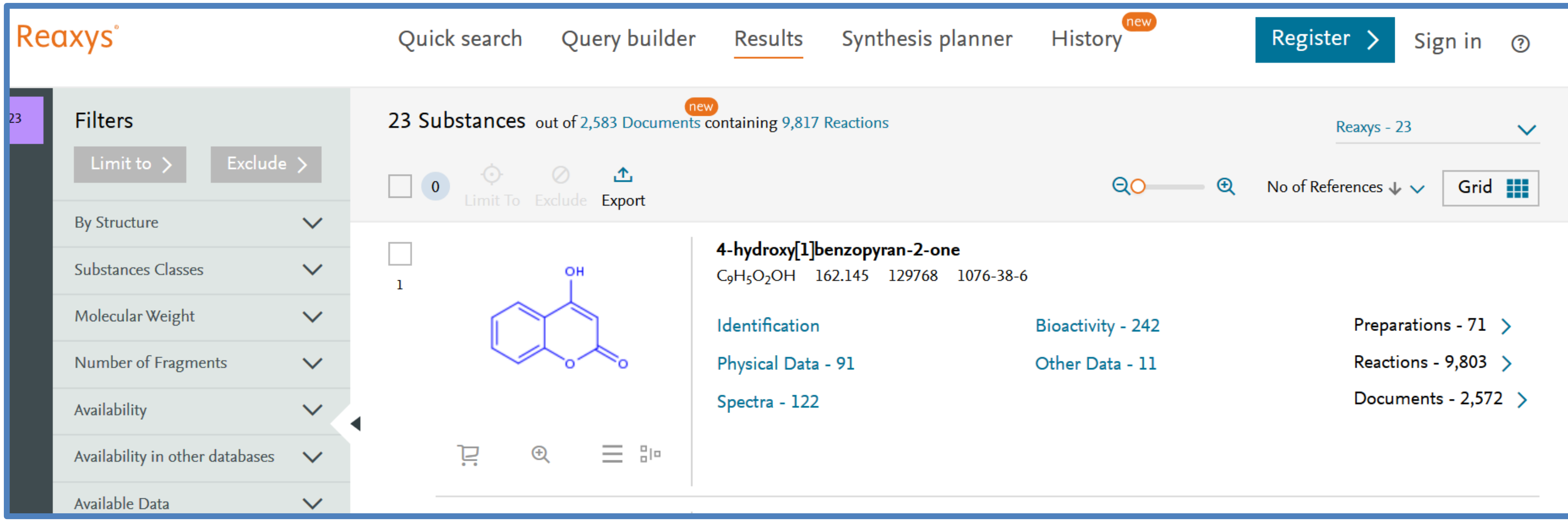
INTRODUCING JOURNAL ARTICLES TO 1st YEAR CHEMISTRY STUDENTS AT KEELE

- ✓ 1st Year Chemistry students generally have no experience of exposure to scientific journal articles
- ✓ Reading journal articles presents challenges for early undergraduates due to the specialist vocabulary, terminology, professional conventions and presumed tacit knowledge.
- ✓ It is therefore necessary to design appropriate activities and assessments that provide opportunities for students to gain the necessary skills required to navigate journal articles and to be able to use them in increasingly sophisticated ways.

1st YEAR CHEMISTRY: SELECTED LEARNING OUTCOMES

Learning Outcomes
✓ Extract and interpret relevant information from scientific literature.
✓ Manipulate and analyse experimental data, using spreadsheets, to create appropriate graphs and extract scientific parameters.
✓ Analyse and interpret ^{1}H and ^{13}C NMR, IR and UV-vis spectra to evaluate the outcome of experimental investigations.
✓ Communicate the outcomes of an experimental investigation via a laboratory report that observes professional practice and conventions in chemistry.
✓ Reflect and act on feedback from a variety of sources.

SELECTED (NON-DISSERTATION) LITERATURE-BASED ASSESSMENTS IN CHEMISTRY AT KEELE



Information Retrieval I

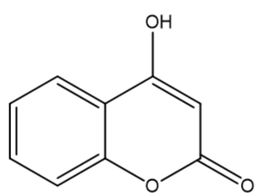


Figure 1: A framework structure of 4-hydroxy[1]benzopyran-2-one[1]

1st YEAR INFORMATION RETRIEVAL EXCERCISES USING REAXYS

Name of compound	4-hydroxy[1]benzopyran-2-one[1]
Molar mass/ $gmol^{-1}$	162.145[1]
Melting point/ °C	208-212[2]
Recrystallisation solvent	Methanol[2]

Table 1: Physical data of 4-hydroxy[1]benzopyran-2-one[1,2].

Frequencies	Assignment
$3380cm^{-1}$	O-H
$1680cm^{-1}$	C=O

Table 2: Principle IR bands with frequencies of 4-hydroxy[1]benzopyran-2-one in the solvent nujol[3].

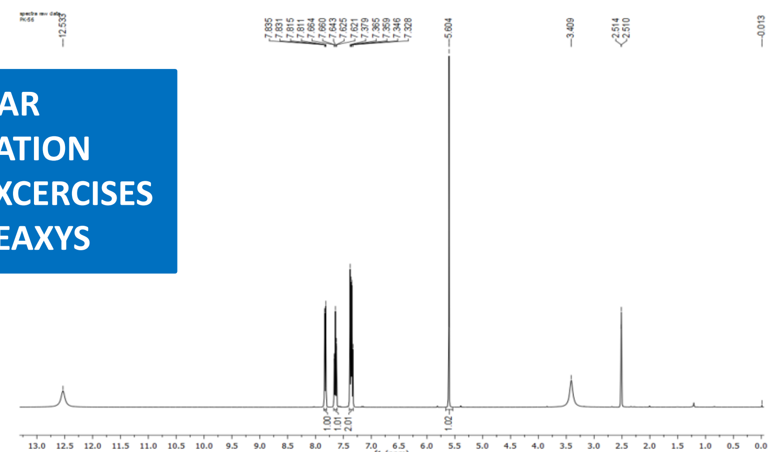


Figure 2: ^{1}H NMR spectra of 4-hydroxy[1]benzopyran-2-one in solvent DMSO-d6[4]

SELECTED (NON-DISSERTATION) LITERATURE-BASED ASSESSMENTS IN CHEMISTRY AT KEELE

3rd YEAR ADVANCED DATA ANALYSIS AND INTERPRETATION BASED ON JOURNAL ARTICLES

CHE- 30038 Portfolio Part 1

1. **Answer are in relation to:** ***J. Am. Chem. Soc.*****, 128, 13611-13624**
   (a) (i) Expression for the equilibrium constant of reaction (1) in the paper in terms of rate constants and estimation of equilibrium constant in toluene at 25°C and atmospheric pressure:

$$2 + NO \underset{k_{off}}{\overset{k_{on}}{\rightleftharpoons}} 2(NO)$$

At equilibrium rates of the forward and reverse reactions are equal.

$$k_{on}[2]_e[NO]_e = k_{off}[2(NO)]_e$$

equilibrium constant, K_{NO} can therefore be expressed as follows:

$$K_{NO} = \frac{[2(NO)]_e}{[2]_e[NO]_e} = \frac{k_{on}}{k_{off}}$$

At 25°C and atmospheric pressure values of rate constants are reported as:

$$k_{on} = 1.80 \times 10^6\ M^{-1}s^{-1}$$

$$k_{off} = 12470\ s^{-1}$$

Therefore:

$$K_{NO} = \frac{1.80 \times 10^6\ M^{-1}s^{-1}}{12470\ s^{-1}}$$

$$K_{NO} = \frac{1.80 \times 10^6\ M^{-1}s^{-1}}{12470\ s^{-1}}$$

$$K_{NO} = +144\ M^{-1}$$

(ii) Estimate ΔH°, ΔS° and ΔG° (at 25 °C) and the equilibrium constant (at 25 °C) for reaction (1).

These parameters are calculated using data from Table 3 from the paper. This is because ΔG° is very temperature dependent, and ΔH° and ΔS° display slight temperature dependence. Thus by using the enthalpies, entropies and free energies of activation from Table 3, more accurate values for ΔH°, ΔS° and ΔG° can be obtained as opposed to using values from Table 2 values for which were gathered by using temperatures between$(-70 - 40)$°C.

Table 1. Calculated parameters corresponding to reaction (1)

Parameters	
ΔH° $(kJ\ mol^{-1})$	−54
ΔS° $(J\ mol^{-1}\ K^{-1})$	−140
ΔG° (at 25 °C) $(kJ\ mol^{-1})$	−13
K (at 25 °C)	+190

Developing Scientific Reporting Skills of Early Undergraduate Chemistry Students

10 Developing Scientific Reporting Skills of Early Undergraduate Chemistry Students

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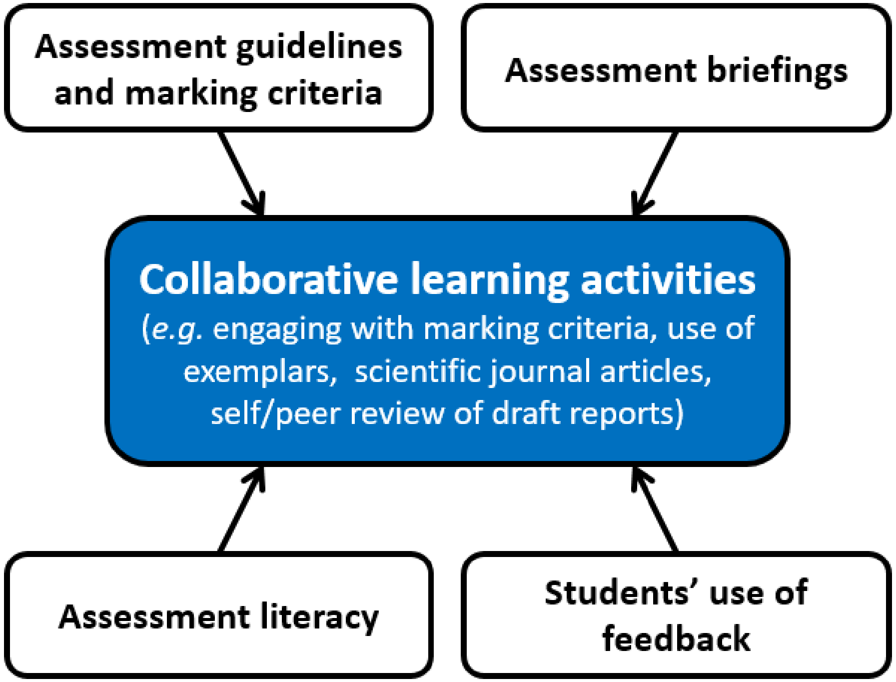
The approach is characterised by a series of iterative assessment-feedback cycles that are supported by scheduled assessment briefing sessions coupled to a range of formative and collaborative learning activities related to aspects of report writing, and deploying journal articles as paradigms of professional practice.

Capel, N. J., Hancock, L. M., Haxton, K. J., Hollamby, M. J., Jones, R. H., Plana, D. and McGarvey, D. J. (2019), “Developing Scientific Reporting Skills of Early Undergraduate Chemistry Students “, in Seery, M. K. and Mc Donnell, C. (Eds.), *Teaching Chemistry in Higher Education: A Festschrift in Honour of Professor Tina Overton*, Trigonal Planar Press, Edinburgh

Dialogic Iterative Approach: Reporting Skills

- ✓ **Authenticity:** journal articles used as paradigms of professional conventions and practice.



- ✓ **Generic (professional) skills**: scientific reporting acts as a vehicle for development of wide-ranging generic (professional) skills.

- ✓ **Assessment-feedback strategy:** spans a full academic year and incorporates many aspects of contemporary thinking surrounding effective assessment-feedback practice, placing strong emphasis on the development of students' assessment literacy and meaningful use of feedback.

CHE-10061: LABORATORY REPORTS

Group Exercise 1:

- ✓ Each group is provided with a set of scientific articles known as '**peer-reviewed scientific papers (or journal articles)**', which have been published in various scientific journals.

- ✓ **Structure:** Scan through the articles and note down the titles of the principal sections of the articles.
- ✓ **Writing style:** How would you describe the writing style?
- ✓ **Referencing:** How is the published work of others and/or other sources of published information cited in the article?
- ✓ **Graphs, illustrations, tables**: How are these presented and what common features are there in the presentation of these?
- ✓ **Equations**: How are these presented?

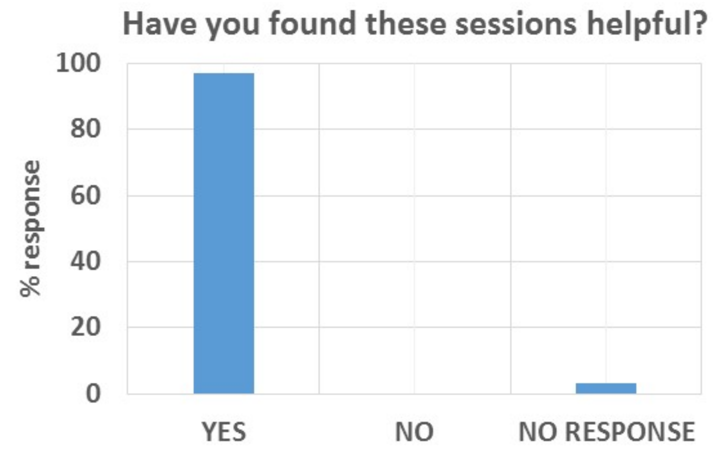
EXERCISE 1: SUMMARY

Article Structure (Principal Sections of Scientific Articles):

- ✓ ***Abstract:*** *A concise synopsis of what is reported, including the principal findings*
- ✓ **Introduction:** Outlines the background to the work, placing it in context and outlines the purpose (aims and objectives) of the work.
- ✓ **Experimental:** Provides the essential experimental details (materials, methods etc.). Papers with synthetic content will include abbreviated spectral data and physical properties.
- ✓ **Results and Discussion:** Presentation of the results/findings and their interpretation.
- ✓ **Conclusion**: A concise summary of the principal findings and how these relate to the aims and objectives. This section may include suggestions for future work
- ✓ **References:** A list of cited sources, formatted according to the referencing system appropriate to the journal.

Assessment Briefing Sessions – Student Feedback

- ✓ **Have you found these sessions helpful (Y/N)**
- ✓ **Please elaborate on your answer and, where appropriate, suggest what could be improved.**



- ✓ ***'They allowed me to understand what was required of me'***
- ✓ *'Ask any questions you had. Look at examples from published papers'*
- ✓ ***'The examples of reports shown were very helpful for generating an idea of how the reports should be structured'***
- ✓ *'Essential, since most have little idea how to write in correct way'*
- ✓ ***'Having an assignment explained in person is much more helpful than reading assessment criteria. Also give the opportunity to ask questions'.***

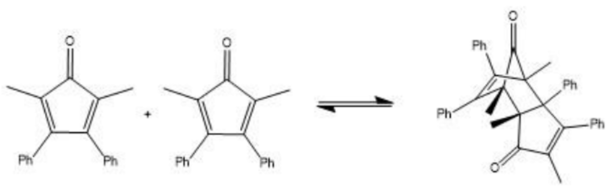
- ✓ *'They helped me to understand the formatting of work. It would be useful to go over the grading criteria in more detail'*
- ✓ *'They introduced the task well ensuring we knew what we had to do and how to achieve our best'*

Scientific Reporting Skills: 1st Year Report Extracts

Temperature Dependence of Equilibrium Constants and the van't Hoff equation

Introduction

The compound 2,5-dimethyl-3,4-diphenyl cyclopentadienone can undergo a reversible dimerization reaction in solution via a Diels-Alder reaction. 2,5-dimethyl-3,4-diphenyl cyclopentadienone exists as a dimer (as seen in Scheme 1) as a solid. However, when this dimer - 'D' - is dissolved in an organic solvent it can, to an extent, spontaneously dissociate into a monomer - 'M' - (as seen in Scheme 1). This dissociation is temperature dependent. As soon as the monomer is formed, an equilibrium will begin to be established and the monomer will react and turn back into the dimer. Once this equilibrium has been determined both the forwards and backwards reactions will progress at the same rate.



(1) - Monomer (1) - Monomer (2) - Dimer

Scheme 1. Reaction of a reversible dimerization of 2,5-dimethyl-3,4-diphenyl cyclopentadienone[1]

Scientific writing

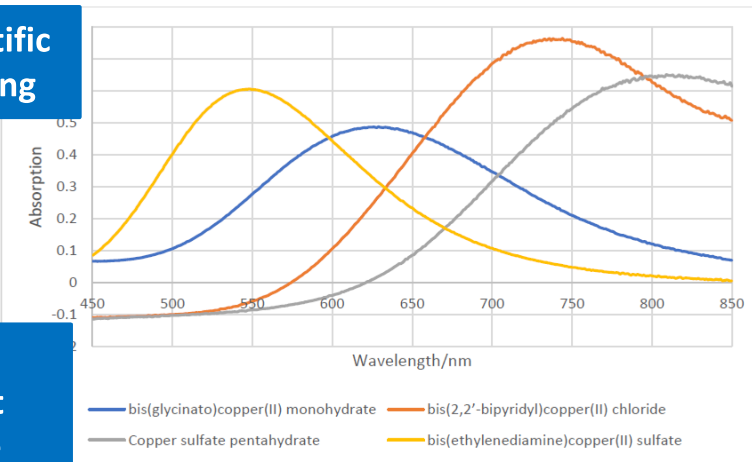


Figure 8. UV-Visible spectrum of the copper complexes

Use of Specialist Software

^{1}H NMR Data: Equation 4 was used to calculate the dissociation of the dimer (α) from the ratio of protons in each environment (R). Equation 3 was then used to calculate the value of K for the solution at each temperature.

Professional Conventions

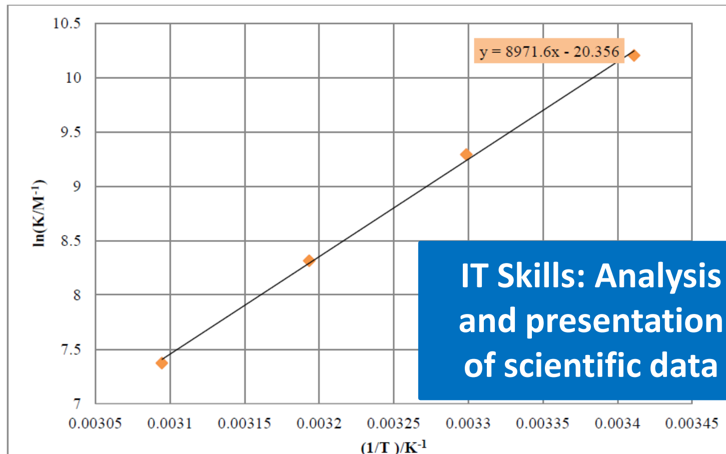
$$\alpha = \frac{R}{(2+R)} \quad (4)$$

$$K = \frac{(1-\alpha)}{4[D]_0\alpha^2} \quad (5)$$

Values obtained experimentally were compared to those from the solution analysed by ^{1}H NMR spectroscopy. Figure 2, a ^{1}H NMR spectrum of the solution at 298K shows five integrated peaks, four of which are from the dimer and one of which is the monomer. This shows the presence of both the reactant and product at equilibrium at the start.

T/K	(1/T)/10^{-3} K^{-1}	[M]$_e$/10^{-3} mol L^{-1}	R/10^{-2}	α/10^{-2}	K/10^{3}M^{-1}	ln(K/M^{-1})
293	3.411	0.679	5.446	2.651	27.063	10.206
303	3.299	1.063	8.661	4.151	10.866	9.293
313	3.193	1.711	14.321	6.682	4.082	8.314
323	3.095	2.682	23.413	10.480	1.592	7.373

Table 1.3- Shows the values calculated using equations 4 and 5 from ^{1}H NMR spectra



IT Skills: Analysis and presentation of scientific data

Figure 3.1- shows the van't hoff plot of the solution analysed by ^{1}H NMR spectroscopy

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3. H M Weiss, *J. Chem. Soc., Perkin Trans. 2*, (1991), 429-443
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Referencing

Scientific Reporting Skills: 1st Year Report Extracts

IT Skills: Analysis and presentation of scientific data

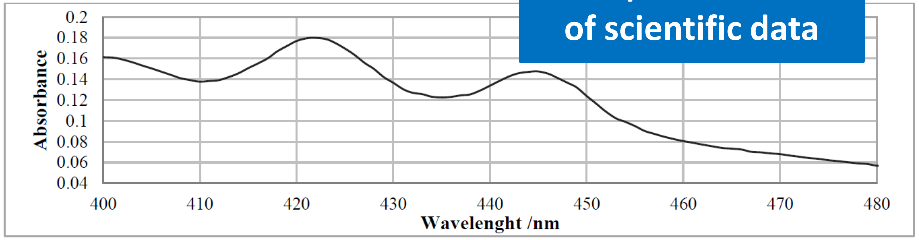


Figure 2: The Visible Absorbance taken of the solution at RT, as shown the absorbance at λ_{max} (422 nm) is 0.18.

The D solution was the placed in water baths at temperatures of 45°C, 55°C, 65°C and 75°C and left to equilibrate for 10 minutes. The absorbance for solutions at each temperature where measured at λ_{max} (422 nm) and used to calculate $[M]_e$ and $[D]_e$ using the molar absorption coefficient (ε = 420 M^{-1} cm^{-1} in t-butanol, lit. [2]). The equilibrium constants (K) for each temperature where then calculated, using equation (1). [1, 9]

T/K	A	$[M]_e$ /mM	$[D]_e$ /mM	K	(1/T) /K^{-1}	lnK
296	0.180	0.429	4.71	25620	0.00338	10.2
318	0.379	0.902	4.47	5491	0.00314	8.61
328	0.708	1.69	4.08	1435	0.00305	7.27
338	1.360	3.24	3.30	315	0.00296	5.75
348	2.032	4.84	2.50	107	0.00287	4.67

Table 1: UV-Visible data, with $[D]_o$ = 4.92 mM, absorbance take at λ_{max} (422 nm) and ε = 420 M^{-1} cm^{-1} lit [2].

The K and T where used to produce the van't Hoff plot (figure 3). This was used with the van't Hoff equation (2), to calculate $\Delta_r H°$ (-91.20 kJ mol^{-1}) and $\Delta_r S°$ (-22.02 J K^{-1} mol^{-1}). [1]

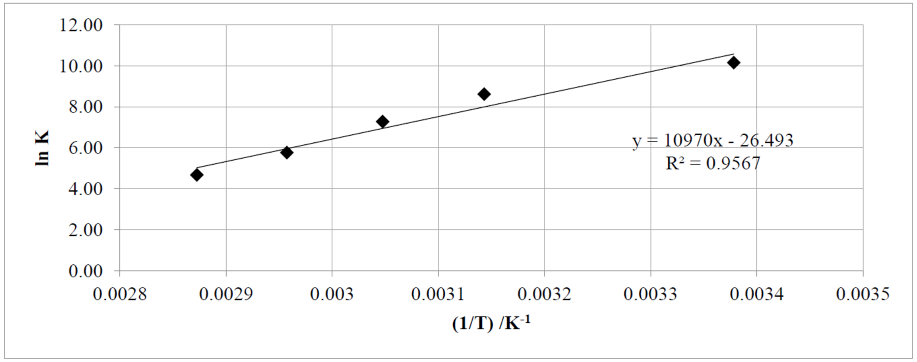
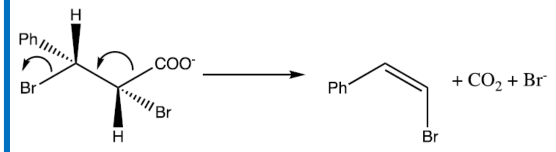


Figure 3: The van't Hoff plot created using the data from the Visible Absorbance data.

Use of Specialist Software



Scheme 2: E2 decarboxylative elimination mechanism of (RS, SR)2,3-dibromo-3-phenylpropanoic acid

IT Skills: Analysis and presentation of scientific data

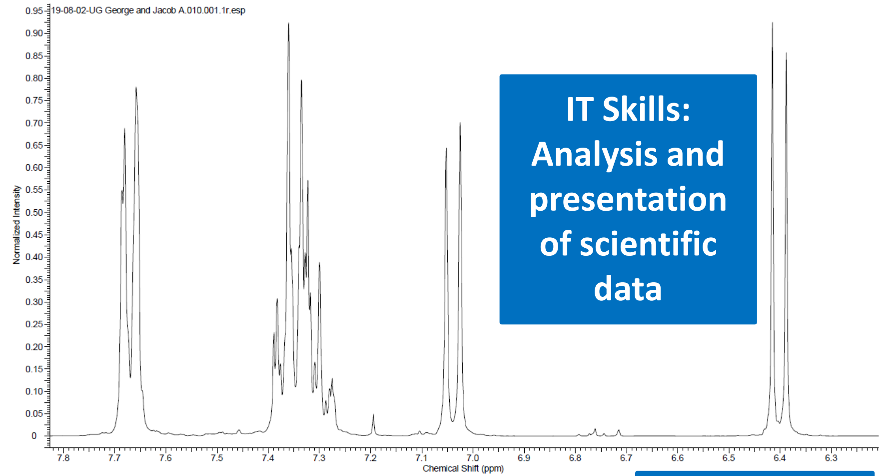


Figure 2: ^{1}H NMR spectrum of beta-bromostyrene following synth

Professional Conventions

Experimental Section

Elimination in Acetone: (RS, SR)2,3-dibromo-3-phenylpropanoic acid (0.6260 g, 2.03 mmol) was dissolved in acetone (10 mL) and K_2CO_3 (0.6197 g, 4.49 mmol) was added. The solution was heated at reflux for 1 h 30 min until the cloudy solution turned white. The solution was cooled to RT and poured onto water (50 mL). The aqueous solution was extracted with diethyl ether (2 × 15 mL), washed with 1 M NaOH (2 × 15 mL) and the solvent removed in vacuo to give pale-yellow oil (0.1607 g, 43%). ^{1}H NMR: δ_H (300 MHz, $CDCl_3$): 7.67 (2H, d, Ar*H*), 7.32 (3H, m, Ar*H*), 7.03 (1H, d, Br-C*H*, $^{3}J_{HH}$ = 8.29 Hz), 6.39 (1H, d, Ph-C*H*, $^{3}J_{HH}$ = 6.00 Hz).

Students' Self-Reporting of use of Feedback

- ✓ Students include statements in the **draft report in semester 2** explaining **how feedback has been used** from **semester 1.**

- ✓ Students include a statement explaining **how feedback from the draft feedback workshop has been used** to improve their final report.

Use of Feedback

I used the feedback to ensure have that my introduction is detailed and contains all the information necessary, including outlining my aims and objectives. I have made sure that figures, tables and equation are introduced in the text and are correctly numbered. I ensured that I reported my data actually and made sure I had the units of the NMR included.

How I used my feedback

I tried to outline the aims of the practical more clearly in the introduction by briefly explaining what I would carry out and how I would use my data in order to link my findings back to the objectives. I also tried to keep the tense the same throughout the report rather than implying I still needed to carry out the experiment.
In my experimental I tried to keep an eye on little details such as capitalising the room temperature abbreviation and making sure the 1 for proton was in superscript.
For the NMR data I would include too much detail and so kept the explanation brief but still contained all the relevant information
Also, in the conclusion I made sure to mention the exact values rather than giving approximates.
I had always references the lab script incorrectly and took the feedback on board in making sure I referenced it as it was a book and included page numbers in the text.

Improvements following the feedback session:

Introduction – I moved the schemes from the results and discussion to the introduction, and removed irrelevant mechanism information so that it was more specific to dependence on solvent. I spoke about $^3J_{HH}$ values in more detail.

Experimental – I removed the NMR data for the minor product in the water section as they are not whole protons. I also tried to specify exactly which proton I was referring to rather than just 'CH_2'.

Results and Discussion – I initially had a synthesis paragraph for both elimination in acetone and water, but I combined these after the feedback session. I also removed all chemical shifts from my spectra, and removed the integrations from the acetone spectrum. I also referred to the $^3J_{HH}$ values in more detail. I mentioned the impurities in each reaction although they are left off the spectra, and mentioned how these may have been present.

Conclusion – I made a suggestion on how to improve the experiment.

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