A Computational Examination of the Effects of Alkali and Alkaline Earth Metals on Hydrogen Atom Abstraction Reactions by Oxygen Centered Radicals

by

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B.Sc. Hons., The University of British Columbia, 2015

A THESIS SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF

MASTER OF SCIENCE

in

THE COLLEGE OF GRADUATE STUDIES

(Chemistry)

THE UNIVERSITY OF BRITISH COLUMBIA

(Okanagan)

June 2017

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The undersigned certify that they have read, and recommend to the College of Graduate Studies for acceptance, a thesis entitled: A COMPUTATIONAL EXAMINATION OF THE EFFECTS OF ALKALI AND ALKALINE EARTH METALS ON HYDROGEN ATOM ABSTRACTION REACTIONS BY OXYGEN CENTERED RADICALS submitted by JEFFREY A. VAN SANTEN in partial fulfilment of the requirements of the degree of Master of Science

Supervisor, Professor (please print name and faculty/school above the	e line)
Supervisory Committee Member, Professor (please print name and fathe line)	aculty/school above
Supervisory Committee Member, Professor (please print name and fathe line)	aculty/school above
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Abstract

This is a sample thesis based on the ubcthesis.cls template from Michael Forbes. The thesis includes the additional style file ubcostyle.sty in accordance to the official standards for the UBCO College of Graduate Studies. This sample thesis together with the style files and templates produces a document that is officially accepted by the UBCO College of Graduate Studies.

If you need a package, look into ubcostyle.sty to see if it is not already loaded there. See the file README.txt for additional instructions to produce the bibliography, index, and glossary automatically.

Preface

Preface stuff

If any part of your thesis was co-written, you must include a Co-Authorship statement. Also indicate if part of the thesis was published with the reference.

Table of Contents

List of Tables

List of Figures

Acknowledgements

This is the place to thank professional colleagues and people who have given you the most help during the course of your graduate work.

Dedication

The dedication is usually quite short, and is a personal rather than an academic recognition. The *Dedication* does not have to be titled, but it must appear in the table of contents. If you want to skip the chapter title but still enter it into the Table of Contents, use this command \chapter[Dedication]{}.

Chapter 1

Introduction

This sample thesis discusses changes from the sample thesis of Michael Forbes, that make the thesis compliant with UBCO College of Graduate Studies standards. If you need more information about the template and LaTeX, please check out the sample thesis of Michael Forbes at

http://alum.mit.edu/www/mforbes/projects/ubcthesis/. [? ? ? ? ? ? ? ?]

1.1 Packages

There are several packages included in ubcostyle.sty. So before you add a new package, check first if it is already included there.

1.2 Glossary

Should you wish to provide a glossary of notation, the ubcostyle file uses the package glossaries. Please read the documentation for this package.

In short, you need to define glossary entries with a keyword at the beginning of the document. You can use the gls with the keyword to add the corresponding page number to the glossary, where the gls command appears. In general, only use this at the place where a symbol or notation is introduced the first time. Sorting can be done with the sort keyword. You can use subgroups (like number sets, operator families, etc.). However, within a group, sorting should be according to appearance in the document.

Once you have all your entries defined, compile your LaTex document. After that, open a command line terminal and cd into the directory of your thesis. If your thesis file name is ubc_2010_spring_doe_jane.tex (which is standard file name required by UBC circle when uploading the thesis), then type

makeglossaries ubc_2010_spring_doe_jane and compile your document again. The glossary should be there.

1.3 Index

Should you wish to provide an index, you need to add commands indexthesis at the appropriate position in your text. Then run the makeindex command as makeindex myfile.idx -t myfile.ilg -o myfile.ind. where myfile is replaced by your filename e.g. ubc_2010_spring_doe_jane-index-glossary

1.4 Epigraph

If you want to add an epigraph to a chapter (epigraph in the sense of a literary inscription, not a function epigraph), you can use the command epigraph after the chapter. Check out the documentation of the epigraph package for more information.

The following are examples of how to incorporate graphics into your thesis.



Figure 1.1: This is a sample figure Note that we have used the optional argument for the caption command so that only a short version of this caption occurs in the list of figures.

You should really put text in between figures so LaTeX has more flexibility to place the figure at the appropriate location.



Figure 1.2: This is the same sample figure with still a long caption but this time we did not use a short caption command in the table of figures.

Table 1.1: Short table title

Table 1.2: Short table title

Table 1.3: Long table title that wraps around several lines and goes on and on and on and on and on

Table 1.4: Short table title

Table 1.5: Short table title

Table 1.6: Short table title

Table 1.7: Short table title

Table 1.8: Short table title





- (a) Figure on the left side is identical to the one on the right.
- (b) Figure on the right side is identical to the one on the left.

Figure 1.3: An example of putting two figures side by side using the subfigure package.

Figure 1.4: Another Figure

Figure 1.5: Another Figure with a very long title to check the alignment in the lof

Figure 1.6: Another Figure

Figure 1.7: Another Figure

Figure 1.8: Another Figure

Figure 1.9: Another Figure

Figure 1.10: Another Figure

Chapter 2

Conclusion

Here comes the conclusion.

I	tem	
Animal	Description	Price (\$)
Gnat	per gram	13.65
	each	0.01
Gnu	stuffed	92.50
Emu	stuffed	33.33
Armadillo	frozen	8.99

Chapter 2. Conclusion

Your conclusion can go on for several pages.

Bibliography

- Aitalioubrahim, M. Commun. Korean Math. Soc. 2011, 26, 515–530.
- [] Azzam-Laouir, D. Electron. J. Qual. Theory Differ. Equ. 2008, No. 37, 9.
- Azzam-Laouir, D.; Izza, S. Comput. Math. Appl. 2011, 62, 1736–1744.
- [] Bačák, M.; Borwein, J. M.; Eberhard, A.; Mordukhovich, B. S. *J. Convex Anal.* **2010**, *17*, 737–763.
- [] Bauschke, H.; Combettes, P. Convex analysis and monotone operator theory in Hilbert spaces; CMS Books in Mathematics / Ouvrages de Mathématiques de la SMC; Springer: New York, 2011; pp xvi+468, With a foreword by Hédy Attouch.
- [] Bernicot, F. Séminaire: Équations aux Dérivées Partielles. 2008–2009; Sémin. Équ. Dériv. Partielles; École Polytech.: Palaiseau, 2010; pp Exp. No. XIX, 13.
- Bauschke, H. H.; Goebel, R.; Lucet, Y.; Wang, X. SIAM J. Optim. **2008**, 19, 768–785.
- [] Bauschke, H.; Goebel, R.; Lucet, Y.; Wang, X. SIAM J. Optim. 2008, 19, 766–785.
- [] Fear, S. Publication quality tables in LaTeX. 2005; http://www.ctan.org/tex-archive/macros/latex/contrib/booktabs/booktabs.pdf.
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- \rightarrow pages

Appendix

- \rightarrow pages
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Appendix A

Tables

Here you can have additional tables. Table captions are always on top. In order to use publication quality tables, one should use the guidelines in [?]. In short, do not use vertical rules or double rules, units in the column heading (not in the body of the table), precede decimals with a digit, and do not use ditto signs. Table ?? is according to the guidelines.

For tables, the caption goes on top, for figures, the caption goes on the bottom. If possible, always position tables and figures at the top of a page.¹ Use the option tbph for the placement.

I	tem	
Animal	Description	Price (\$)
Gnat	per gram	13.65
	each	0.01
Gnu	stuffed	92.50
Emu	stuffed	33.33
Armadillo	frozen	8.99

¹In this case, the chapter heading prevents the table from being at the top.

Table A.2: Another table

Table A.3: Another table

And other table materials (I needed to generate two pages for that appendix to test the formatting of the table of content).

Table A.5: Another table

Table A.6: Another table

Table A.7: Another table

Table A.8: Another table

Table A.9: Another table

Table A.10: Another table

Table A.11: Another table

Appendix B

Figures

Here you can have additional figures. Figure captions are always at the bottom.

Appendix B. Figures

And other additional figures (again I needed to generate two pages :-).