

Instructions for writing a scientific thesis

1 INTRODUCTION

These instructions apply to B.Sc. thesis, B.Sc. project report, M.Sc. (pro gradu) thesis and licentiate thesis. It may also be used as guidance for laboratory reports. For Ph.D. thesis university level instructions are applied.

These instructions aim at defining the layout of the thesis and clarifying some other practicalities related to thesis writing. Instructions are not imperative and they can be applied and deviated in collaboration with a supervisor still keeping in mind the clarity of the thesis. Wording, unity and clarity of the thesis (including abbreviations, references and layout of tables and figures) are important parts of the thesis. Special attention should be paid on language.

There is no definite rule for the length of the thesis; it depends on the topic. The general rule, however, is that a B.Sc. thesis should contain 15-20 references and around 15-25 pages of text. A M.Sc. thesis should have around 50 references and 50-80 pages of text and a licentiate thesis should contain 100-200 references and 80-100 pages.

The experimental part (a project report and an experimental part of a M.Sc. thesis) should include the theoretical background of the work, methods and materials used, information about the experimental work described so that any chemist with a similar background could repeat the experiments and measurements.

2 GENERAL CONTENT OF THE THESIS

The thesis should contain the following parts:

- A. Cover page
- B. Abstract
- C. Preface
- D. Table of contents
- E. Abbreviations
- F. Introduction
- F. The main text divided into a literature part and an experimental part
- G. Conclusions / Summary
- H. Literature / References
- I. Appendices (if any)

- A.** An example of the cover page is presented in Appendix 1
- B.** The abstract summarizes the aims and the results of the work shortly (max. 1 page). A reader should get a clear idea about the contents of the work. The abstract page does not contain any other text.
- C.** The preface / foreword (max. 1 page) presents where and when the work was done, if it was done in collaboration with the industry or other third parties and who were the supervisors of the work. Also other practicalities related to the work can be presented. The definition of the topic and how the material was obtained may also be commented. The preface ends with the acknowledgements.
- D.** The table of contents presents the structure of the thesis with chapter and page numbering (Appendix 2).
- E.** A list of abbreviations and symbols used in the text with explanations. The page listing the abbreviations does not contain any other text. In the main text, the abbreviation is

explained to a reader when it is mentioned for the first time. For example: “Capillar electrophoresis (CE) is a method...”

- F.** The main text contains a literature part and an experimental part, unless there is a specific reason separate them as individual works (e.g. industrial collaboration, separate topics) (Appendix 2).

The thesis begins with an **Introduction**, in which the topic is introduced on a general level. After that the literature and theory of the topic are gone through in the *literature part* followed by an *experimental part*. In the experimental part methods, equipment, reagents and results are presented. Pay attention to the accuracy of the presentation and analysis. The experimental part can be presented either in the form of an article manuscript or as a report. The whole text should be logical and clear. Please use sub-headings to clarify.

Conclusions / Summary ends the thesis and compiles the most important aspects and results. The significance of the results, whether the goals were achieved and how the research could be continued are also commented. This part is similar to the abstract but broader and more detailed. If the experimental part is written in the form of an article manuscript, the description of the experimental procedures is usually presented after the conclusions (e.g. detailed synthesis instructions).

- G.** The references are presented after the main text and before the appendices. See details for presenting the references in Ch. 3.6.
- H.** Selected appendices help to understand the results and analysis, but are such that they are not reasonable to present in the text (large tables, spectral data, measurement series etc.). See Ch. 3.3.

3 LAYOUT AND TYPOGRAPHY

3.1 General layout

The thesis is written in the size A4 with following margins: left and right 2.5 cm; top 2.5 cm, and bottom 1.5 cm. The page number (header) is placed in the middle the top of the page. The font is Times New Roman (or equal) 12 pt and line spacing 1.5. The headings may also be the size of 14 pt. Coloured fonts or headings are not used.

Instructions for LaTeX are presented in Appendix 3.

3.2 Chapters and sections

The sections and chapters are not indented, but the text is justified. The sections are separated with an empty line and the chapters with two empty lines. The headings and molecular numbers are written with **boldface**. In the numbering of the chapters and sections no more than four numbers are used (e.g. 3.2.1.1). Emphasised parts (if needed) can be marked with *italics* or underline.

3.3 Figures and tables

The most important figures and tables should be included in the text. Additional figures and tables may be included as appendices. Pay attention to the layout of the tables: they should not be too dense, large or contain too much information.

Figures, tables, reaction equations, compounds and schemes are numbered. Figures and their captions are centered and the figure caption is presented under the figure (one empty line between the figure and caption). Tables and table captions are aligned left and separated from the main text by an empty line. Table captions are presented above the table. The text of the figures and tables is written with a normal font with few exceptions (e.g. Latin names, other exceptions generally written in italics). The figure captions end with a full stop, but the table captions do not.

The main text should have a reference to each figure and table. The reference is usually presented in parenthesis in the end of the sentence, which addresses the topic of the figure or table. For example: “This sentence tells about the contents of the figure 1 (Figure 1).” If the figure or table is taken directly from a reference, the caption should have a reference to the original literature and the permission for reproduction should be asked from the publisher.

For example:

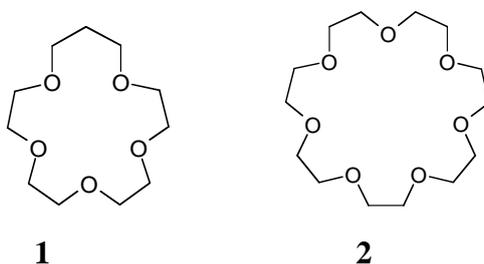


Figure 1. Two crown ethers, 16-Crown-5 (**1**)² and 21-crown-7 (**2**).³

Each value / information presented in a table should have a heading row or heading column, in which also the unit of the value is presented. The values are presented with a reasonable accuracy and errors / standard deviations are presented without exception, if possible. 15 unit rule is used for rounding. A large table can be presented in landscape orientation, but the table cannot be divided into two pages except for exceptional cases. Footnotes may be used to clarify the contents of a table and the font size of a footnote may be smaller, for example 10 pt. The layout of the table should be clear and simple and the same style should be used throughout the thesis.

For example:

Table 1. Standard molecular entropy $S^O(298\text{ K})$ of some compounds and elements⁴

Substance (standard state at 298 K)	$S^O(298\text{ K}) / \text{J mol}^{-1}\text{K}^{-1}$
Ag (crystalline)*	42.6
C (graphite)	5.7
C (diamond)	2.4
Fe (crystalline)	27.3
I ₂ (crystalline)	116.1
HBr (gas)	198.7
PCl ₃ (liquid)	217.1

*This is an explanation for silver.

3.4 Page numbering

- The cover page is not numbered.
- The pages presenting the abstract, the preface, the table of contents and the abbreviations are numbered with small roman numbers: i, ii, iii, iv, v....
- The main text pages are numbered with 1, 2, 3...
- The appendices are numbered with APPENDIX 1, APPENDIX 2... and the numbers are located on the top right corner of the page.

3.5 Tenses

A passive voice and the same tense are used logically throughout the text. In the experimental part, when presenting one's own work, passive imperfect is used '*The reaction mixture was stirred for six hours*'. If the results of others are presented, the tense is passive perfect: "...*have presented*...". General conclusions and generally known fact is presented in present tense: "The results show that the concentration increases...".

3.6 References

Each fact presented in the text that is not a generally known should have a reference to the original and preferably the first publication about the topic (so called primary reference; book, scientific article, presentation etc), of which the reader can find more information about the topic. In some cases it is justified to use a reference that is easier to find or published later than the first one (the original article is written in unusual language, it is published in a book that cannot be obtained etc.). The references are marked with running numbers and superscripts after the sentence addressing the topic.

For example: This is an example, which is based on several references.^{7,11-15,23}

If the whole section is based on one reference or the section is compiled from several references, the reference(s) can be presented in the end of the section. The reference number can also be placed in other positions in the text.

For example: The earlier studies show that the compounds can be used as a cancer medicine,⁷ medical materials,⁸ conductive materials¹⁰ and in analytics¹¹.

If the name of the author is mentioned in the text, the reference is placed immediately after the name.

For example:

- i) If there is only one author: “Shimada² has observed...”
- ii) If there are two authors: “Armarego and Reece¹ have observed...”
- iii) If there are three or more authors: “Knabe *et al.*⁸ have observed...”

Note! *et al.* is usually written in italics.

If the topic is relatively common and could be found in various references, only one of the references can be chosen.

For example: “As generally known (see for example ref. 7)...”

The list of references should contain sufficient information for a reader to find the original reference. Special attention should be paid to the names of the authors, the titles of the articles and bibliographical information. The list of references should contain the names of all authors, i.e. *et al.* cannot be used in the list of references. All references are presented in a uniform style.

It is highly recommended to use RefWorks, Mendeley or equivalent reference manager program. Also reference management of the word processor can be used. Department of Chemistry and University library organize courses for using reference managers and databases, and searching information.

3.6.1 Scientific articles as references

1. A running number and full stop.
2. The complete last name, the initial letter(s) of the first name(s) of the author(s), possible Jr. or Sr, separated with a comma. If there are more than two authors, the names of the authors are separated with semicolon.

For example: Kilmberg, M., Jr.; Klimberg, M. A., Sr.; Stilton, D. and Rehn, O.

3. The name of the article as it is written. The general rule is that the words of the title are written without capital first letters, except for the first word. Depending on the chosen reference style the title of the article is not necessarily shown. Consult your supervisor if the titles are needed or not.
4. The name of the journal is written with *italics*. The names of the journals are abbreviated according to CAS Source Indexin (CASSI; cassi.cas.org).
5. The year in **boldface**, space, *volume number in italics*, the first and the last page number separated with a hyphen and full stop. Note! Some journals do not have a volume number (for example some RSC publications). The issue number is presented only if the page numbering in each issue of a volume is started from 1.

For example: *J. Appl. Cryst.*, **1994**, 27, 4-11.

6. If the original journal is not available or published with an unusual language, an English abstract (if available) can be used as a reference (see Example 2 below). The source of the abstract should be presented. Generally, however, it is recommended to use the original reference.

Examples

1. Armarego, W. L. F. and Reece, M., Quinazolines XXV. The synthesis of 8-chloro-2-[4-(2-furoyl)-piperazin-1-yl]-6,7-dimethoxyquinazolin-4-amine hydrochloride (8-chloroprazosin hydrochloride), *Aust. J. Chem.*, **1981**, *34*, 1561-1566.
2. Shimada, K., Organic compounds in kraft bleaching spent liquors. V. Photodegradation of red-pine chlorinated oxygignin, *Mokuzai Gakkaishi*, **1982**, *28*, 376-382. *Chem. Abstr.*, **1983**, *97*, 129328v.
3. von Weizmann, G. Kubel, H. ja Lange, W., Untersuchungen zur Cancerogenität von Holzstaub. Die Extraktstoffe von Eichenholz (*Quercus robur* L.), *Holzforsch.*, **1989**, *43*, 75-82.

3.6.2 Books and theses (M.Sc. or Ph.D. thesis) as references

1. A running number and full stop.
2. The name(s) of the author(s) as written in the references to scientific articles. If a book is a collection of articles/chapters written by different authors and with an editor, both the author(s) and the editor are mentioned. (see example 8 below)
3. The name of the book in italics.
4. The edition (if not the 1st), the publisher, the place of printing, country, the year of publishing.
5. The first and the last page number, for example pp. 19-31. If the whole book is a reference, no page numbers are needed.
6. If the different parts of the same book are used as a reference, the different parts are separated with a letter in a reference. See example 6 below.

Examples

4. Kivinen A. and Mäkitie O., *Kemia*, 3. ed., Otava, Keuruu, 1981, pp. 23-35.
5. Ebersson, L., *Organisk kemi*, Almquist & Wiksel Förlag AB, Stockholm, Sweden, 1969.
6. Sjöström, E., *Wood Chemistry - Fundamentals and Applications*, 2. ed., Academic Press, San Diego, USA, 1993. a) pp. 2-14 b) 67-84 c) 101-104.
7. Jeffrey G. A. and Saenger, W., *Hydrogen Bonding in Biological Structures*, 2. ed., Springer-Verlag, Berlin, Germany, 1994.

8. Dence, C. W., The determination of lignin, in Lin S. Y. and Dence C. W. (eds.), *Methods in Lignin Chemistry*, Springer-Verlag, Berlin, Germany, 1992, pp. 32-61.
9. Kotoneva, J., *Steroidit supramolekulaarisessa kemiassa*, M. Sc. thesis, University of Jyväskylä, Department of Chemistry, Jyväskylä, 1995.
10. Leppänen, J., *Design and Synthesis of Entacapone Prodrugs and L-Dopa – Entacapone Codrugs*, Kuopio University Publications A. Pharmaceutical Sciences 59, Ph.D. thesis, University of Kuopio, Faculty of Pharmacy, Department of Pharmaceutical Chemistry, Kuopio, 2002.

3.6.3 Presentations or posters as references

Oral and poster presentations are sometimes published as a compilation or an abstract book (for example Conference Proceedings or Proceedings, abbreviated as *Conf. Proc.* or *Proc.*). When these are used as a reference the time, the place and the organiser of the conference are given. Typical abbreviations used in this context are *Int.* or *Intl.* = International) and *Symp.* = symposium. For example *Int. Symp. Pulping Chemistry*.

Examples:

11. Hyötyläinen, J., Characterization of lignin and humic compounds in receiving water system of pulp industry. Use of model compounds and CuO-oxidation-HPLC-method, *Conf. Proc. TOCEON 93, Toxic Compounds in Environment, Znojmo, Czech Republic*, 1.-3.6.1993, pp. 78-84.
12. Ristolainen, M. and Alén, R., Characterization of effluents from TFC bleaching of hardwood kraft pulp, *Proc. 1996 Int. Pulp Bleaching Conf.*, Book 2, Washington, D.C., USA, 14.-18.4.1996, TAPPI Press, Atlanta, USA, 1996, pp. 523-525.

3.6.4 Other references

Unofficial sources: Other references, that should be mentioned, can include essential but unofficial sources, such as an interview with an expert or e-mail correspondence with an expert.

Examples:

13. Paasivirta, J., oral statement 24.7.1996.
14. Nissinen, M., e-mail correspondence, 14.3.2010.

Computer programmes: If a non-trivial, but essential computer programme is used in the work a reference should be given. The name of the programme is written with capital letters. Many scientific programmes used in research have their own, specific reference. The reference is placed immediately after the name of the programme.

Examples:

15. Sheldrick, G. M., *SHELXL-97 - A program for crystal structure refinement*, University of Göttingen, Germany, 1997.
16. Sheldrick, G. M., *Acta Crystallogr., Sect. A: Found. Crystallogr.* **2008**, 64, 112-122.

Patents:

17. Kanbe, S., Shinazaki, Y. ja Takei, K., Substituted phenyl benzoates and their use in liquid crystal composition, *Ger. Offen*, 3,001,423, 26.1.1979.
18. Pystynen, J., Luiro, A., Lotta, T., Ovaska, M. ja Vidgren, J., Cathecol derivatives, *US Pat.*, 6,150,412, 2000.

A series of a research institute or a university:

19. Tuominen, I., MILOX-prosessin kemikaalitaseen tarkastelu tuotantomittakaavassa, PSC Communications 80, 28.8.1995, Oy Keskuslaboratorio- Centrallaboratorium Ab, 1995.

WWW-pages: A direct address of the www page can be given, if the address is informative and fully traceable. The date when the reference was taken must be given in the parenthesis at the end of the reference.

For example:

20. High Performance Liquid Chromatography (HPLC): A Users Guide, <http://www.pharm.uky.edu/ASRG/HPLC/hplcmytry.html>, University of Kentucky, The Advanced Science and Technology Commercialization Centre, Analytical Spectroscopy Research Group (15.4.2002).

3.7 Nomenclature of chemical substances and structures

Chemical substances and formula are named according to IUPAC rules. When the substance is mentioned for the first time, formula or schematic picture of a compound should also be given, unless the compound is generally known (for example water). Trivial names may be used if the name is in general use (for example acetone), but it may also be clarified with a systematic name, when mentioned for the first time. With large and complicated systems it may not be reasonable to use IUPAC names. In those cases an agreed abbreviation or a number presented in the scheme of the structure should be used. The chemical structures are drawn with a special program, such as ChemDraw, using an ACS style or similar.

3.8. Units and quantities

Units and quantities are given in SI-units. Acceptable exceptions are: Celsius degree °C, litre (l), Ångström (Å), minute (min), hour (h), day (d), year (a), wave number (cm^{-1}) and electron volt (eV).

3.9 Specific instructions

There may be some subject specific instructions and practises available. Consult your supervisor. For experimental work there are specific instructions related to laboratory safety.

4 OTHER INSTRUCTIONS

A written contract about the M.Sc. thesis should be made in Korppi in agreement with the student and supervisor. The purpose of the contract is to agree about the schedule and supervisors of the thesis and ensure that both the student and the supervisor(s) are committed to the thesis. Evaluation criteria of the thesis should be looked through when the contract is made.

The procedure of writing the literature part starts with collecting and familiarising with the material. The material is sorted and a table of contents is drafted and presented to the supervisor. The table of contents is a frame of the work and will be corrected and completed during the process. It is strongly recommended that a regular schedule for meetings with the supervisor is agreed. The purpose of the meetings is to follow up the progress of the work and provide answers to the problems during the writing of the thesis. An efficient writing of a thesis takes time and requires concentration. The experimental part is about 16 weeks of full-time laboratory work (Mon-Tue 8-16). It is not recommended to take many simultaneous courses and studies during the thesis. It is recommended to write experimental part already when the work is in progress and the topic is still fresh in mind.

In questions concerning technical details, layout and other issues related to thesis it may be beneficial to look through some of the earlier thesis done in the research group or at the department. Electronic versions of M.Sc. theses can be found from Jyväskylä University Digital Archive JYX (<https://jyx.jyu.fi/>).

The thesis, which is left for grading, is inspected with Urkund plagiarism checker. The thesis is sent to the analysis address of the supervisor after which the supervisor gets a report, which is included in the evaluation. The student may ask a copy of a report from the supervisor. For more information: <https://www.jyu.fi/itp/en/plagiarismdetection> .

APPENDIX 1

Title of the thesis

M.Sc. thesis

University of Jyväskylä

Department of Chemistry

xx.xx.xxxx

Rihanna Researcher

APPENDIX 2

TABLE OF CONTENTS

ABSTRACT	i
PREFACE	ii
TABLE OF CONTENTS	iii
ABBREVIATIONS	iv
<u>LITERATURE PART</u>	
1 INTRODUCTION	1
2 ALCOHOLS AND ETHERS AS GUEST MOLECULES	3
2.1 MONOALCOHOLS	3
2.2 DIOLS	8
2.3 POLYOLS	10
2.3.1 Complexes of alkyl resorcinarenes and polyols	10
2.3.1.1 Exceptional examples	11
<u>EXPERIMENTAL PART</u>	
9 EQUIPMENT AND MATERIALS	52
10 PROTECTION OF ALDEHYDES	55
10.1 PROTECTION REAGENTS	56
13 CONCLUSIONS	75
14 SYNTHESIS INSTRUCTIONS	77
16 REFERENCES	90
APPENDICES	

APPENDIX 3

Instructions for using LaTeX

Those using LaTeX may use common sense in layout. Please follow the general instructions on the order of presentation and aim for a clear layout. The page layout of LaTeX is usable as it is, but may be changed closer to these instructions.

Examples of settings to start with:

```
\documentclass[a4paper , 12pt , english]{report} %tai article
\usepackage[T1]{fontenc}
\usepackage[latin1]{inputenc}
\usepackage[english]{babel}
\usepackage{overcite}
\usepackage[dvips]{graphicx}
\linespread{1.5}

\begin {document}

\parindent0pt
\parskip3mm
\pagestyle{headings}

\newcommand{\frontmatter}{\pagenumbering{roman}}
\newcommand{\mainmatter}{\newpage%
  \pagenumbering{arabic}%
  \setcounter{page}{1}}
\newcommand{\backmatter}{}
\setcounter{page}{1}

\begin{titlepage}
  \vspace*{6cm}
  \begin{center}
    \Huge{Title}
  \end{center}
  \vfill
  \begin{flushright}
    Pro gradu thesis \\
    University of Jyväskylä \\
    Department of Chemistry \\
    31.12.2050 \\
    Stan Student
  \end{flushright}
\end{titlepage}
\frontmatter
%starts the page numbering with roman numbers

\include{abstract}

\include{preface}
```

`\include{abbreviations}`

APPENDIX 3 (CONTINUED)

`\pagebreak`

`\tableofcontents`

`\pagebreak`

`\mainmatter`

%starts the page numbering with normal numbers

`\include{introduction}`

`\include{text}`

`\include{more text}`

`\include{still more text}`

`\include{so much more text}`

`\include{Conclusions}`

`\addcontentsline{toc}{chapter}{Literature/references}`

`\bibliographystyle{unsrt}`

`\bibliography{ref}`

`\end {document}`