

# Christoph's Template for Writing a Dissertation with L<sup>A</sup>T<sub>E</sub>X

Christophs Vorlage zum Schreiben von  
Dissertationen mit L<sup>A</sup>T<sub>E</sub>X

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**(Dr. rer. nat.)**

Vorgelegte

**Dissertation**

VON

**Yourname Here**

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## **§8 Abs 1 lit. d PromO**

Ich versichere hiermit, dass zu einem vorherigen Zeitpunkt noch keine Promotion versucht wurde.

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# Zusammenfassung

Dieses Dokument soll künftigen Doktoranden als  $\text{\LaTeX}$  Vorlage für Dissertationen dienen und enthält Hinweise und Beispiele, von denen ich mir gewünscht hätte sie im Voraus zu wissen. Ich hoffe es hilft euch, aber ich kann weder für Richtigkeit noch Nützlichkeit garantieren. Ich werde davon ausgehen, dass ihr bereits mit grundlegenden  $\text{\LaTeX}$ -Funktionen vertraut seid. An manchen Stellen wird man, anstatt nur das pdf zu lesen, in den Quellcode schauen müssen um die Vorlage sinnvoll nutzen zu können. Zum Beispiel die Titelseiten (Titelseite, bibliographische Informationen, Promotionsordnung) haben einige auskommentierte Hinweise im  $\text{\LaTeX}$  Code zu den formalen Anforderungen und dem Hochladen auf TUprints. Diese Hinweise wollte ich nicht im PDF erscheinen lassen, damit sie für eine echte Dissertation nicht gelöscht werden müssen. Oft habe ich versucht den entsprechenden  $\text{\LaTeX}$  Code direkt im PDF erscheinen zu lassen, sodass ihr ihn (fast direkt, Vorsicht vor zusätzlichen Leerzeichen) copy-pasten könnt, und eine Beispielanwendung mitzuliefern. Ich selbst habe mich zu Beginn auch an einer Sammlung von Hinweisen zur  $\text{\LaTeX}$ -Dissertationen orientiert, die ich im Internet gefunden habe, schaut gerne auch dort vorbei: <http://alexanderfabisch.github.io/latex-for-dissertations.html>  
Stand 2023-03-22.

## Abstract

This document is meant as a  $\text{\LaTeX}$  template to help future PhD students write their dissertations and contains notes and examples which I would have liked to know in advance. I hope it helps, but cannot guarantee that I got everything right. I will assume that you are familiar with the basic functions of  $\text{\LaTeX}$ . In some cases, you will need to look at the source code rather than the pdf to make sense of the template. For instance, the title pages (title page, bibliographic information, Promotionsordnung) contain some commented notes in the  $\text{\LaTeX}$  code regarding the formal requirements and upload to TUprints. I did not want these notes to appear in the pdf such you don't need to delete them in your actual dissertation. I often tried to display the  $\text{\LaTeX}$  code in the pdf, so you can copy and paste it (nearly as is, mind additional whitespaces), and also provide an example of what it looks like in practice. I myself took initial advice from a collection of notes for  $\text{\LaTeX}$  dissertations I found on the internet, you are encouraged to also

visit: <http://alexanderfabisch.github.io/latex-for-dissertations.html> as of  
2023-03-22.

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# Part I. Parts Only Serve Demonstration Purposes Here

## 1. Spacing

### 1.1. Special Spacing for The First Chapter in a Given Part

Here is how to save space by avoiding a pagebreak between a new part and its first chapter:

---

```
\begingroup
%save space by avoiding a pagebreak between a new part and its first chapter
\renewcommand{\cleardoublepage}{}%only necessary if the openright option is
    used in the documentclass options. Otherwise only acting on \clearpage is
    sufficient, but renewing also \cleardoublepage does no harm.
\renewcommand{\clearpage}{}
\chapter{Spacing}
\endgroup%reinstate normal function of the clearpage commands
```

### 1.2. Margins

I tried to get the current margin sizes for even and odd pages, so I can set new custom margin sizes to adjust for the binding. The macro you find below prints a short text which describes left and right margins and whether the code thinks that it is currently on an odd or even page (relevant to grant more space to the binding). You can then jump to the next page (which is then the other of odd or even) and let it give you the margin sizes there. This did not work fully for me (odd / even page recognition failed), but at least it worked for either an even or an odd page, which was good enough for me.

---

```
%get margins
%https://tex.stackexchange.com/questions/537078/how-to-access-geometry-length
\usepackage{ifoddpage}% subsequent commands need the siunitx package. If you
    use the code from the steckexchange link, be sure not to keep the siunitx
    package options given there for your final version, otherwise all values of
```

## 1. Spacing

```
the \SI command will be given with the specified (two-decimal) precision,
which sucks if you cannot make such a precise statement or only wanted to
get a consistently formatted order of magnitude. Made this mistake and got
over-precise polymer content (\SI{4}{\wtpercent} yielded "4.00 wt%" instead
of "4 wt%") or completely wrong output (\SI{e7}{\hertz} yielded ".0010-7
Hz" instead of "10-7 Hz").

\makeatletter
% Macro for nicely printing a length in centimeters. You don't need it to *use*
the lengths.
\newcommand*{\convertToCm}[1]{%
  \begingroup
  \edef\tmp{\strip@pt\dimexpr(#1)/7227*254\relax}%
  \SI{\tmp}{\centi\meter}%
  \endgroup
}
\makeatother
\newlength{\myLeftMargin}
\newlength{\myRightMargin}
\newcommand*{\myComputeMargins}{% To be called just after \checkoddpages
  \setlength{\myLeftMargin}{%
    \dimexpr 1in + \ifoddpages\oddsidemargin\else\evensidemargin\fi
  \relax}%
  \setlength{\myRightMargin}{%
    \dimexpr \paperwidth - \textwidth - \myLeftMargin \relax}%
}
\newcommand*{\myMarginCheck}{%this command did not differentiate between even
and odd page for me, but was nonetheless useful to figure out how large the
margin is
  \checkoddpages\myComputeMargins
  This is an \ifoddpages odd\else even\fi page. The left margin is thus
an
  \ifoddpages inner\else outer\fi one and its width is
  \the\myLeftMargin, that is \convertToCm{\myLeftMargin}. The right
margin is
  \the\myRightMargin, that is \convertToCm{\myRightMargin}.\par
}
```

---

```
Example usage:\\
\myMarginCheck
\newpage
\myMarginCheck
```

Example usage:

This is an even page. The left margin is thus an outer one and its width is 79.09862pt, that is 2.7789 cm. The right margin is 100.15381pt, that is 3.51917 cm.

This is an even page. The left margin is thus an outer one and its width is 79.09862pt, that is 2.7789 cm. The right margin is 100.15381pt, that is 3.519 17 cm.

## 2. References with `\cref`

### 2.1. Simple Uses of `\cref`

I assume you are familiar with the basic `\label` and `\ref` functionality of L<sup>A</sup>T<sub>E</sub>X. Let me just add that there is the `\cref` command from the `cleveref` package, which automatically detects the environment (e.g. chapter, subsection, equation) it is used in. This comes in handy if you want to convert, say, a section into a chapter. If you simply always used `\cref`, you don't need to find all instances like "As mentioned in sec. `\ref{test}`" and adjust them to "As mentioned in chap. `\ref{test}`".

### 2.2. Highlighting References

You can highlight references as document-internal links one can click on to jump to the corresponding page of the document. Commonly, the `hyperref` package is used for that, whereby I found customizing the following package options useful:

```
\usepackage{hyperref}%package options are handled with the hypersetup command
\hypersetup{
    colorlinks    = true, %Colours links instead of ugly boxes. hidelinks
    option removes boxes but then does not highlight links at all
    %            hidelinks, %un-comment to suppress link colors for the print
    version. Note that this does not have the "option=true/false" syntax.
    urlcolor      = blue, %Colour for external hyperlinks
    linkcolor     = blue, %Colour of internal links
    citecolor     = red,  %Colour of citations
    plainpages    = false,%so that hyperref treats page ii and page 2 as
    separate pages, https://tex.stackexchange.com/questions/93889/why-does-backref-refer-to-wrong-page
    pdfpagelabels,%glossary pagenumbers get offset by 1 per \part, at least
    when I also mess with clearpage commands. trying solution of https://tex.stackexchange.com/questions/21698/how-to-get-correct-glossary-links-with-frontmatter-pages
}
```

Highlighting links is nice for the electronic version, but does not make sense for the printed dissertation. To disable link-colours, you can conveniently use the "hidelinks" option. Note that `hidelinks` is not set to e.g. "true" or "false", you just write "hidelinks" and move on to the next package option.

The `cleveref` package should be loaded after any package without specific support for `cleveref`. It is safest to load it at the very end of the preamble. You may or may not want to use the `[nameinlink]` option to include/exclude reference types (equation, section etc.) in `hyperlink`. `nameinlink` appears to be too recent for the current installation on my office computer (as of 2024-12-17).

---

```
Example usage:\\
%
Reference a section, cf. \cref{sec:cleveref_simple}. Here is a reference to two
  figures at once: \cref{fig:binodal-spinodal-phase-diagram,fig:
    energylevelszeeman-qp1}\\.\\
%
Here is a reference of two different things (a section and a table) at once: \
  cref{sec:polym_concentration_dependences,tab:list-of-samples}. And a
  reference to three subsequent sections \cref{sec:first_cycle,sec:
    ageing_days,sec:ageing_hours}.
```

---

Example usage:

Reference a section, cf. sec. 2.1. Here is a reference to two figures at once: figs. 8.1 and 8.3. Here is a reference of two different things (a section and a table) at once: chap. 2 and table 9.1. And a reference to three subsequent sections secs. 2.1 to 2.3.

## 2.3. Advanced Uses of `\cref`

This part stems from a niche use case I was too stubborn to let go of: I wanted to be able to reference a set of subequations (say, equations 1a) and 1b)), whereby the (abbreviated) word for the reference type would signal a plural “eqs.” although only the common equation number is displayed, i.e. “eqs. 1)”. With the default configuration, I could only manage things like “eqs. 1a) and 1b)”. On the road I also picked up how to change the referencing labels in general, so maybe this helps you:

---

```
%customize abbreviations of e.g. section and chapter references. You probably
  don't want to repeat this with the capitalizing version, \Crefname, as
  abbreviations at the beginning of a sentence apparently are considered bad
  style.
%crefname command structure: \crefname{type}{singular}{plural}
\crefname{equation}{eq.}{eqs.}
\crefname{section}{sec.}{secs.}
\crefname{chapter}{chap.}{chaps.}
%
%How to make a plural-reference to a set of subequations with a single label.
%Originally I tried the solution from this link: https://tex.stackexchange.com/
  questions/35772/referencing-subequations-with-cleveref
%unfortunately, Multi-references also require all the other cross-reference
  formats to be defined, so I redefined those as well. A brief explanation of
  the command structures:
```

---

## 2. References with `\cref`

```
%crefformat arguments: #1=formatted label counter, #2=start of hyperlink, #3=
end of hyperlink
%crefmultiformat arguments: \crefmultiformat{type}{format for the first cross-
reference in a list of multiple cross-references}{format for the second
cross-reference in a list of two cross-references}{format for any middle (
not first or last) cross-reference in a list of more than two cross-
references}{format for the last cross-reference in a list of more than two
cross-references}
\crefformat{equation}{eq.~(#2#1#3)}
\Crefformat{equation}{Eq.~(#2#1#3)}%
\crefmultiformat{equation}{eqs.~(#2#1#3)}{ and~(#2#1#3)}{, (#2#1#3)}{ and
~(#2#1#3)}
\crefformat{section}{sec.~#2#1#3}%crefformat overwrites at least the singular
from crefname
\Crefformat{section}{Section~#2#1#3}%explicitly define \Crefformat, instead of
using the default (\MakeUppercase together with \crefformat) because
abbreviations at the beginning of a sentence are bad style.
%\crefrangeformat{section}{secs.~(#3#1#4) and~(#5#2#6)}
\crefmultiformat{section}{secs.~#2#1#3}{ and~#2#1#3}{, #2#1#3}{ and~#2#1#3}
%Note that there is also \crefrangemultiformat, which I however did not need to
specify
\crefformat{chapter}{chap.~#2#1#3}
\Crefformat{chapter}{Chapter~#2#1#3}
\crefmultiformat{chapter}{chaps.~#2#1#3}{ and~#2#1#3}{, #2#1#3}{ and~#2#1#3}
\crefformat{figure}{fig.~#2#1#3}%crefformat overwrites at least the singular
from crefname
\Crefformat{figure}{Figure~#2#1#3}%explicitly define \Crefformat, instead of
using the default (\MakeUppercase together with \crefformat) because
abbreviations at the beginning of a sentence are bad style.
%\crefrangeformat{figure}{figs.~(#3#1#4) and~(#5#2#6)}
\crefmultiformat{figure}{figs.~#2#1#3}{ and~#2#1#3}{, #2#1#3}{ and~#2#1#3}
```

### 3. Citations

I used biblatex and found customizing the following package options and additions useful:

```
\usepackage[
style=alphabetic,% with this style citations in the text are based on author
names. Other people may prefer the style ‘‘numeric’’
maxnames=2,%sets maximum number of names in citations for both intext (
maxcitenames) as well as bibliography. If there are more authors, your
settings for abbreviating lists of authors in citations, i.e. ‘‘minnames’’
kick in
maxalphanames=2,%not sure what max|minalphanames do differently from max|
mincitenames, but if I use them it looks like I want it to.
minalphanames=1,
minnames=1,%if number of names in citation is larger than maxnames, cut after
minnames-many names and add ‘+’
maxbibnames=99,%overwrite maximum number of names befor truncations in
bibliography
uniquelist=true,%allows deviations from maxnames to make lists unique
backref,%references the pages where the citation was used
%url=false,%url can be set to false to ignore the url-fields of the .bib file.
I did not want to generically throw away urls here, because I want to cite
e.g. the grace-website. URLs are handled below.
]{biblatex}

\usepackage{xurl}% load after biblatex. Avoids URLs of references reaching into
the margin. see https://tex.stackexchange.com/questions/686510/break-line-in-bibliography-for-doi

%avoid references with (chemicals in) titles reaching into the margins by
manually adding discretionary hyphens (\-) in the affected entries of the .
bib file. see https://tex.stackexchange.com/questions/381542/article-title-not-linebreaking-correctly-in-bibliography

%failed to have bibliography in two columns, with the title as for a onecolumn
page. Contending myself with smaller font to keep required space reasonable.
Feel free to try yourself, maybe one of these links help:
%https://tex.stackexchange.com/questions/137100/two-columns-10pt-bibliography-specific-pages-only-in-a-one-column-12pt-text
\appto{\bibfont}{\small}%onecolumn, normal fontsize: 40 pages. small: 32 pages.
footnotesize: 28 pages
%\appto{\bibsetup}{\raggedright\twocolumn}
```

### 3. Citations

```
%\AtEndBibliography{\onecolumn}
%https://tex.stackexchange.com/questions/20758/bibliography-in-two-columns-
%section-title-in-one
%\usepackage{multicol}
%\usepackage{etoolbox}
%\patchcmd{\thebibliography}{\section*{\refname}}
%{\begin{multicols}{2}[\section*{\refname}]}{}{}
%{\patchcmd{\endthebibliography}{\endlist}{\endlist\end{multicols}}{}{}}

\AtBeginRefsection{\GenRefcontextData{sorting=ynt}}%ensure that (also) a ynt
sorted refcontext is created
\AtEveryCite{\localrefcontext[sorting=ynt]}%use the ynt refcontext for sorting
within a citation. Did not trust this and sorted references manually, if
there were multiple references in a single citation command

\addbibresource{/autohome/saeckech/Seafire/Sync_Seafire/Literatur_Promotion/
Library/Promotion_Literatur.bib}%(path for office computer)

%do not cite fields like 'comment' in the bibliography
\AtEveryBibitem{%
  \clearfield{note}%
  % \clearfield{url}%handled below
  \clearfield{eprint}%
  \clearfield{isbn}%
  \clearfield{issn}%
  \clearfield{month}%
  \clearfield{abstract}%
  \clearfield{creationdate}%
  \clearfield{pages}%
  \clearfield{file}%
  \clearfield{issue}%
  \clearfield{number}%
  \clearfield{keywords}%
  \clearfield{numpages}%
  \clearfield{printed}%
  \clearfield{ranking}%
  \clearfield{readstatus}%
  \clearfield{edition}%did not enter edition for every book and want to
keep output consistent. Also, output formatting for first editions ("First")
is for some reason different from other editions ("2nd ed.")
}
% want to show specific URLs only. Solution stolen from: https://tex.
stackexchange.com/questions/152869/show-url-only-for-one-reference,
2024-11-04
%create a new category, for which the URL will be printed in the references
\DeclareBibliographyCategory{needsurl}
\newcommand{\entryneedsurl}[1]{\addtocategory{needsurl}{#1}}
\renewbibmacro*{url+urldate}{%
  \ifcategory{needsurl}
```



```

        {\printfield{url}%
         \iffielddundef{urlyear}
         {}
         {\setunit*{\addspace}%
          \printurldate}}
    {}
}
%manually set bib-entries which should have their URL printed in the references
%with the new ‘‘entryneedsurl’’ command defined above. Example:
\entryneedsurl{PubChem2005NIPAM}

```

---

Example usage: Basic citation `\autocite{Halperin2015}`, citation with a page number `\autocite[2]{Halperin2015}`, multiple basic citations `\autocite{Fujishige1989, Halperin2015, Korde2019}`, multiple citations with a page number `\autocites[1]{Fujishige1989}[1]{Halperin2015}`, citations with a mentioned author `\textcite{Halperin2015}` and multiple citations with mentioned authors each `\textcite{Halperin2015, Korde2019}.\`

%  
The following citation should keep its URLs in the bibliography `\autocite{PubChem2005NIPAM}`.

Example usage: Basic citation [Hal+15], citation with a page number [Sli90, p. 2], multiple basic citations [Fuj+89; Hal+15; KK19], multiple citations with a page number [Fuj+89, p. 1; Hal+15, p. 1], citations with a mentioned author Halperin et al. [Hal+15] and multiple citations with mentioned authors each Halperin et al. [Hal+15] and Korde and Kandasubramanian [KK19].

The following citation should keep its URLs in the bibliography [Pub].

Recall that you may need to compile the bibliography (and potentially the glossary, if you use one) separately from the “normal” L<sup>A</sup>T<sub>E</sub>X compiling, especially if you want to update the pagenumbers (“backref option”) on which the references were cited. If you use Textstudio as editor, you can compile the bibliography via Tools→Bibliography (F8 key by default).

When talking about the *Carr-Purcell-Meiboom-Gill* (CPMG) pulse sequence, I wanted to make sure that both authors of both publications are explicitly named with the `\textcite` command. The document-wide settings for how many names are to be mentioned may, however, differ. I therefore used a variable “globalmaxnames” for the document-wide settings (not included in the example code of chap. 3, but you can check the actual source code), then set the number of names to 2 directly before the citations, then set the number of names back to the document default

---

```

Example usage: The \CPMG sequence, originally devised by \
setmaxcitenames{2}\textcite{Carr1954}\setmaxcitenames{\globalmaxnames} %
setmaxcitenames to 2 (even though it is the current (2025-04-10) default)
to ensure that both Carr and Purcell are mentioned by name
and later improved upon by \setmaxcitenames{2}\textcite{Meiboom1958}\
setmaxcitenames{\globalmaxnames}%setmaxcitenames to 2 (even though it is

```

### 3. Citations

```
the current (2025-04-10) default) to ensure that both Meiboom and Gill are
mentioned by name
    , repeatedly refocusses dephasing spins
```

Example usage: The [CPMG](#) sequence, originally devised by Carr and Purcell [[CP54](#)] and later improved upon by Meiboom and Gill [[MG58](#)], repeatedly refocusses dephasing spins.

## 4. Glossary

Glossaries are quite some work to get running, but I think they are worth it in the end. I hope this chapter reduces the work you need to put in until it works the ways you want it to. Feel free to simply use my `glossary.tex` file, but be aware that it contains some customization and editing based on my personal preferences.

Why should you use a glossary in the first place? Maybe less so for what you classically expect from a glossary (to look up the meanings of words in a list at the end of a book), but rather to make sure that acronyms and symbols are properly introduced. For instance, you want to tell the reader what *poly(N-isopropylacrylamide)* (pNIPAM) is the first time you mention it, but from there on by default only use the abbreviation pNIPAM. But what if you later rearrange your sections? Sure, you can manually search for the text where you originally introduced the abbreviation and edit it, but that is annoying and there is a risk you overlook some such word at some point. If you use the glossary package, it will handle this for you. If required, you can also manually tell L<sup>A</sup>T<sub>E</sub>X to use the term as if it had not been used before (example in source code: *poly(N-isopropylacrylamide)* (pNIPAM)). For instance, I wanted to make sure that *Carr-Purcell-Meiboom-Gill* (CPMG) is spelled out when I explain what it is in the experimental details section, even though I might have mentioned it previously. To do so, I used a custom modification of the package-included `\genacrfullformat` command (and similar for grammatical variations):

```
\newcommand{\fakefirstacr}[1]{\ifglused{#1}{\glsdisp{#1}{\genacrfullformat
{#1}}}{\gls{#1}}}%manually set an acronym to be displayed as if it was its
first use, in order to have the long forms displayed e.g. in the conclusion
to give clarity to readers which only read the conclusion. Dont want to
simply reset uses, such that occurrence counts are kept and thus document-
wide single-uses do not have a redundant abbreviation introduced
```

For non-acronyms, there was no need to count how often they occur in total (cf sec. 4.1). To simply reset the glossary’s internal tracker for “did I use this before?”, a glossary-package-included command, `\glsreset`, is available. With it, you can e.g. mention in you abstract which range of *Larmor frequencies* ( $\omega_L$ ) you measured but then have the *Larmor frequency* ( $\omega_L$ ) treated as a novel term when you mention it for the first time in your theory section.

Glossaries can, in principle, also handle symbols with a special symbol-glossary, but I just messed with my existing glossary instead, e.g. for the hydrodynamic radius ( $R_h$ ), which I can subsequently use in the text (example: hydrodynamic radius) without introducing the symbol again. Note: If you do so, make sure that you use the same symbol,  $R_h$ , in actual math environments, e.g. via:

#### 4. Glossary

---

```
\newcommand{\Rh}{\ensuremath{R_{\mathrm{h}}}}%hydrodynamic radius
\newglossaryentry{Rh}{name=hydrodynamic radius, first=hydrodynamic radius \
  textnormal{(\Rh)}, prefixfirst={a\ }, prefix={an\ }, plural=hydrodynamic
  radii, type=unignored, description={}, user1={off}}
```

---

You can easily adjust glossary terms for grammar, i.e. plural form and/or capital first letter (for this example I suppress the function that the abbreviation should only be introduced on the first occurrence by resetting any possible prior use of the glossary term “LCST” via `\glsreset{LCST}`):

---

```
Example usage: \gls{LCST}\glsreset{LCST}, \Gls{LCST}\glsreset{LCST}, \glspl{
  LCST}\glsreset{LCST}, \Glspl{LCST}\glsreset{LCST}
```

---

Example usage: *lower critical solution temperature* (LCST), *Lower critical solution temperature* (LCST), *lower critical solution temperatures* (LCSTs), *Lower critical solution temperatures* (LCSTs).

The default plural form simply appends an “s” to the term, but you can set the plural form to something else when you create the glossary entry:

---

```
\newglossaryentry{spectral density}{name=spectral density, plural=spectral
  densities, type=ignored, description={}, user1={off}}
Example usage: \glspl{spectral density}\glsreset{spectral density} instead of \
  gls{spectral density}s
```

---

Example usage: *spectral densities* instead of *spectral densitys*.

Also, the article before the term (“a” or “an”) may depend on whether the long or the short form follows, which can also be handled by the glossary. To have this article functionality, you need at least the “glossaries-prefix” package, instead of the “glossaries” package. I did in fact use the glossaries-prefix package, however, in hindsight, I should have used the “glossaries-extra” package, which provides even more useful (professional) functionalities, for which I had to sometimes create messy custom solutions. To use a glossary term with its article, use the “`\pgls`” command or its grammatical variations like `\Pgls`.

---

```
\newacronym[
prefixfirst={a\ },%prefix used on first use
prefix={an\ }%prefix used on subsequent use
]{LCST}{LCST}{lower critical solution temperature}
Example usage: \glsreset{LCST} first use with article \pgls{LCST} and
  subsequent use with article \pgls{LCST} and grammatical variation \Pgls{
  LCST}.
```

---

Example usage: first use with article a *lower critical solution temperature* (LCST) and subsequent use with article an *LCST* and grammatical variation An *LCST*.

#### 4.1. Special Cases Depending on Acronym Occurrence Counts

I created a custom glossary (I called it the “ignored” glossary because it does not list the words it contains at the end of the thesis) to get special formatting (here: italic) for uncommon words (which are not acronyms) the first time they occur, for instance when I describe what an *athermal* solvent is. When I speak of an athermal solvent the next time, I want normal formatting. Again, you could manually change the font, e.g. to italic (or better: use `\emph` to highlight the word by giving it *italic* typeface in normal cases, and roman typeface if the surrounding text is already italic), but you run into the same problems as for acronyms when you rearrange your sections.

Later on, I changed my mind on which words I consider highlight-worthy, but I had already used the glossary-command structure for every occurrence of the word, so I could not simply remove the corresponding glossary entry without heaving to find and replace every occurrence in the code (annoying) – and what if I later changed my mind again? So I created another, very similar glossary type (I called it the “unignored” glossary), which allows me to keep the command structure, but does not apply any special formatting.

You can also make L<sup>A</sup>T<sub>E</sub>X behave as if it was using the glossary term while displaying something else. This made sense for me as I defined a glossary entry for “*complexation*”, but maybe first mention solvent “*complexes*”, which refers to the same idea but is beyond a simple grammar variation. With the “`\glsdisp{complexation}{complexes}`” command, I can let L<sup>A</sup>T<sub>E</sub>X know that I refer to the idea of complexation without making separate entries for every possible related case.

Also, I wanted different formatting (italic long form, roman short form) for acronyms, so I created a custom acronym style which you can see in the glossary.tex file if you are interested.

### 4.1. Special Cases Depending on Acronym Occurrence Counts

The basic glossary functions can already handle many cases. Depending on your ambitions, however, it can get complicated: Say you have an acronym, “test single-use acronym”, which you use only once in the entire document, then it neither makes sense to introduce the abbreviation nor to create a link to the list of acronyms at the end of the thesis.

You can account for such a case by using the flag “`\glsenableentrycount`” (place before `\begin{document}`), which counts the occurrences of the corresponding glossary command (may need two compile runs, which you probably do anyways, maybe even without knowing). Then use “`\cgls`” commands instead of “`\gls`”. If you don't feel like typing an extra letter in the command, or don't want to replace a bunch of `\gls` commands you already used, you can redefine the `\gls` commands to function like the `\cgls` commands via “`\let\gls\cgls`” and similarly for the other grammatical versions like the plural `\glspl` command.

## 4. Glossary

### 4.1.1. Extra Special Cases Depending on Acronym Occurrence Counts

For even more complexity, counting occurrences gets messed up by glossary resets. I initially wanted to reset all the glossaries after the abstracts (both after the German and the English abstract each) and prior to the conclusion. This way, the acronyms would be re-introduced together with their long forms in the main part and in the conclusion, which readers may find helpful if they skip the abstract and/or only read the conclusion. But what happens when, say, an acronym occurs several times in the main part, but only once in the conclusion? If you aren't careful with the glossary reset, this will be considered as a single occurrence in the conclusion and thus not get an abbreviation or link to the list of acronyms at the end of the thesis. Catching such cases apparently can be done automatically, but seemed to be more effort than I wanted to invest for these fringe cases. Instead, I wrote code which forces a like-first-use style when applied to an acronym and manually applied it to relevant occurrences of acronyms in the conclusion when it was close to the final version.

To test it, here is more than one mention of *test multiple-use single in conclusion* (TMUSC), TMUSC in the main text. See also part II.

In theory, similar issues arise if an acronym is mentioned exactly once in the abstract(s) and exactly once in the rest of the document (main part and conclusion combined), but I just hoped that this would never be the case.

Recall that you may need to compile the glossary (and potentially the bibliography, especially if you use the “backref” option) separately from the “normal” L<sup>A</sup>T<sub>E</sub>X compiling, especially if you want to update the pagenumbers (“backref option”) on which the references were cited or when you care about occurrence counts. If you use Texstudio as editor, you can compile the glossary via Tools→Glossary (F9 key by default).

## 5. Macros

“Macros” may sound more complex than it needs to be. Sure, you can make it very elaborate, but you can also get a lot of value without getting too involved. You can think of macros as commands, which tell  $\text{\LaTeX}$  to do some specific thing you previously defined. For a very simple example, this can save you some typing for long words or annoying commands, i.e. I can define a command “ $\backslash\text{ctg}$ ” which makes  $\text{\LaTeX}$  spell out “coil-to-globule transition” in the pdf wherever I type “ $\backslash\text{ctg}$ ” in the code. To do so, I would create the command via:

---

```
 $\backslash\text{newcommand}\{\backslash\text{ctg}\}\{\text{coil-to-globule transition}\}$ 
```

Example usage: From then on,  $\backslash\text{mbox}\{\backslash\text{textbackslash}\text{ctg}\}$  is available:  $\backslash\text{ctg}$

Example usage: From then on,  $\backslash\text{ctg}$  is available: coil-to-globule transition.

These macros may also contain other  $\text{\LaTeX}$  commands, i.e. just like above I can define a command “ $\backslash\text{pNIPAM}$ ” which triggers the corresponding glossary entry:

---

```
 $\backslash\text{newcommand}\{\backslash\text{pNIPAM}\}\{\backslash\text{gls}\{\text{pNIPAM}\}\backslash\text{xspace}\}$ 
```

Although with such very simple macros, I can only make use of one of the glossary grammar cases (here the basic  $\backslash\text{gls}$  for singular and non-capitalized first letter)

It is considered good practice (which I myself did rarely adhere to) to use the “starred version” of the  $\backslash\text{newcommand}$  command.

Be aware that  $\text{\LaTeX}$  usually does not print the whitespace after a command in the code. For instance, using the  $\backslash\text{ctg}$  command mentioned above, I might want to have it followed directly (without a whitespace) by the character “s” to make the word a plural. To do so, I would write as code

---

```
 $\backslash\text{ctg}\text{ s}$ 
```

Example usage:  $\backslash\text{ctg}\text{ s}$

Example usage: coil-to-globule transitions.

If I mistakenly wrote as code “ $\backslash\text{ctgs}$ ”,  $\text{\LaTeX}$  would try to find my definition of the command “ $\backslash\text{ctgs}$ ” which probably does not exist or has a different function.

Alternatively, I might want to write a separate word next. To do so, I could write as code

---

```
 $\backslash\text{Example usage: }\backslash\text{ctg}\backslash\text{space is a series of words}$ 
```

## 5. Macros

Example usage: coil-to-globule transition is a series of words.

This works but it is clunky. People are lazy and invented the `xspace` package which provides the `\xspace` command, which automatically decides whether a whitespace should be printed. This way I could simply append `\xspace` to most of my custom commands. If you want to get rid of this automatic whitespace for a given use, you can use the `\unskip` command, i.e.

---

```
\newcommand*{\ctgnew}{coil-to-globule transition\xspace}
Example usage: \ctgnew say something \ctgnew\unskip s \ctgnew \ctgnew, (mind
the non-whitespace between commands and before interpunctation) \ctgnew1
```

---

Example usage: coil-to-globule transition say something coil-to-globule transitions coil-to-globule transition coil-to-globule transition, (mind the non-whitespace between commands and before interpunctation) coil-to-globule transition 1.

## 5.1. Typesetting

### 5.1.1. Actual Notes on Typesetting

#### Indices

Although it is not what this section is meant to be about, you can read up on the use of italic vs roman font in scientific context here: <https://iupac.org/wp-content/uploads/2016/01/ICTNS-On-the-use-of-italic-and-roman-fonts-for-symbols-in-scientific-text.pdf>.

#### Units

Most readers of this template will already know the `siunitx` package. Therefore I just briefly mention here that custom units can be defined and options to style the expression to your liking exist, e.g.

---

```
\DeclareSIUnit{\wtpercent}{wt\%}
Example usage: \SI{1}{\wtpercent}, \si{\wtpercent}, $\leq\SI[per-mode=
reciprocal-positive-first]{1}{\mole\square\meter\per\second\per\kilogram}$
```

---

Example usage: 1 wt%, wt%,  $\leq 1 \text{ mol m}^2 \text{ s}^{-1} \text{ kg}^{-1}$ .

It seems to be considered better practice to use the `\qty` commands, because the command name “SI” is awkward if you use a non-SI unit, see <https://tex.stackexchange.com/questions/603217/should-i-use-qty-or-si-for-siunitx>. However, as of this writing, the `\qty` behaves weirdly (maybe it clashes with the physics package?), so I cannot provide examples. Curiously, while `\SIrange` does not work, `\qtyrange` does:

---

```
Example usage: \qtyrange{1}{2}{\wtpercent}
```

---



Example usage: 1 wt% to 2 wt%.

I did not know until now that the `\Srange` or `\qtyrange` commands exist and they would have come in handy for me while writing the dissertation. You can probably also customize package options of the `qtyrange` commands to your liking, i.e. e.g. to either use a format like “1 wt% to 2 wt%” or like “1 – 2 wt%”.

### Dashes and Space Between “e.g.”

A few somewhat out-of-context remarks which I didn’t yet find a better place to mention: You may also want to be aware of the difference of a single minus - in the latex text environment vs double minus – which looks slightly different.

Thin spaces in the German “z. B.” apparently aren’t a thing in English. Depending on your language and setup, you may want to add

---

```
\frenchspacing%avoid double whitespace after ‘.’, usefull in abbreviations e.
g. ‘e.g.’
```

to your preamble.

### Odds and Ends

---

```
%avoid single empty lines (called widows and orphans) on paragraph- or
pagestart and -end
\clubpenalty=10000% penalizes orphans
\widowpenalty=10000% penalizes widows
\displaywidowpenalty=10000% penalizes widows that are immediately
followed by a formula \[ ... \]
\usepackage{microtype}%supposedly more visually appealing borders of
the textblocks%needs scalable fonts, therefore may not work on all machines.
However, it deals well with (avoiding) line breaks and respecting the
margins e.g. for macros
\usepackage[parfill]{parskip}%controls indentation after linebreak and
todonotes. https://tex.stackexchange.com/questions/74170/have-new-line-
between-paragraphs-no-indentation
```

### Textsuperscript <sup>2</sup>H vs Math Mode <sup>2</sup>H

In section titles, you probably want to use `\textsuperscript{2}H` to type <sup>2</sup>H in order to keep the section-header font. Similar for subscripts.

#### 5.1.2. Macros for Typesetting

More towards the purpose of this template, in this section I wanted to suggest you think about the use of macros to keep your options open about typesetting and naming. Of course, this cannot reasonably be done for every word you ever type, but makes sense

## 5. Macros

in some cases: For instance, if you are not yet sure which symbol to use for the Larmor frequency (maybe  $\omega_L$ ,  $\omega_{\text{L}}$  or  $\omega_0$ ) and whether or not the possible “L” in the index should be italic or roman (maybe you know this one, but what about italic vs roman regarding the axis of a spin  $\hat{I}_z$  or rank and order of a spherical harmonic  $Y_l^m$ ?), you could use

---

```
\newcommand{\wL}{\ensuremath{\omega_{\mathrm{L}}}}
```

---

and, if you or a higher power have a change of mind, you can later change what the command does to

---

```
\newcommand{\wL}{\ensuremath{\omega_0}}
```

---

As another example, you could use

---

```
\newcommand{\qpAsym}{\ensuremath{\eta}}
```

---

for the asymmetry parameter of quadrupolar coupling. If you later find that you also want to speak of viscosity or other coupling asymmetry parameters (maybe chemical shift), which conventionally go with the the same symbol,  $\eta$ , you can simply change what the command `\qpAsym` does to e.g.

---

```
\newcommand{\qpAsym}{\ensuremath{\eta_{\mathrm{Q}}}}
```

---

Third example: there are packages (`mchem` or `chemformula`) to write chemistry-stuff with L<sup>A</sup>T<sub>E</sub>X. For the little chemistry we usually need to write in the physics department, a simple macro will do

---

```
\newcommand*\chem[1]{\ensuremath{\mathrm{\#1}}}%math mode to allow subscripts as
in $H_2O$. Could also have used \textsubscript instead. Use a macro to
penalize hyphenation and easily unify (and possibly change) typesetting.
Big packages like mchem or chemformula are a bit overkill for me.
%
Example usage: Here is a chemical: \chem{NaNO_3^-}
```

---

Example usage: Here is a chemical:  $\text{NaNO}_3^-$ .

You cannot define the same command twice, i.e.

---

```
\newcommand{\qpAsym}{\ensuremath{\eta}}
%possibly write a lot of text with a lot of uses of \qpAsym which you don't
want to find and edit.
\newcommand{\qpAsym}{\ensuremath{\eta_{\mathrm{Q}}}}
```

---

would give you an error. However, you can change what a command does mid-document with the `\renewcommand` command:

---

```
Example usage:\\
\newcommand{\qpAsym}{\ensuremath{\eta}\xspace}%
This \qpAsym is \qpAsym a \qpAsym line \qpAsym of \qpAsym text \qpAsym.\\
\renewcommand{\qpAsym}{\ensuremath{\eta}\xspace}%
This \qpAsym is \qpAsym a \qpAsym line \qpAsym of \qpAsym text \qpAsym
```

---

Example usage:

This  $\eta$  is  $\eta$  a  $\eta$  line  $\eta$  of  $\eta$  text  $\eta$ .

This  $\eta_Q$  is  $\eta_Q$  a  $\eta_Q$  line  $\eta_Q$  of  $\eta_Q$  text  $\eta_Q$ .

In this example it does not make much sense to change what `\qpAsym` does in the middle of your thesis, but your use case might well be different. Admittedly, most of the time I used `\renewcommand`, it was in order to mess with predefined functionalities of other packages. For instance, to avoid pagebreaks between the headings of a part and the first chapter in it, see sec. 1.1.

## Row Vectors

If you want to save vertical space while writing a vector, you could use a (transposed) row vector. To be honest, I don't understand the code myself (it seems to require the `xparse` package), but here is where I got it from and what it is:

<https://tex.stackexchange.com/questions/39051/typesetting-a-row-vector> as of 2024-10-22

---

```
\ExplSyntaxOn
\NewDocumentCommand{\Rowvec}{ O{,} m }
{
    \vector_main:nnnn { p } { & } { #1 } { #2 }
}
\NewDocumentCommand{\Colvec}{ O{,} m }
{
    \vector_main:nnnn { p } { \ } { #1 } { #2 }
}

\seq_new:N \l__vector_arg_seq
\cs_new_protected:Npn \vector_main:nnnn #1 #2 #3 #4
{
    \seq_set_split:Nnn \l__vector_arg_seq { #3 } { #4 }
    \begin{#1matrix}
        \seq_use:Nnnn \l__vector_arg_seq { #2 } { #2 } { #2 }
    \end{#1matrix}
}
\ExplSyntaxOff
%Optional transpose macro:
\newcommand{\Transpose}{\ensuremath{\mathrm{T}}\xspace}
```

---

You can then use this as follows

---

```
Example usage:
\begin{equation}\label{eq:b1-rotating}
    \bm{B}_1(t) = B_1 \Rowvec{;}{\cos(\omega_{\mathrm{rf}} t + \varphi_{\mathrm{rf}}), -\sin(\omega_{\mathrm{rf}} t + \varphi_{\mathrm{rf}}), 0}\Transpose\eqend{.}
\end{equation}
```

---

## 5. Macros

which is even more handy for footnotes<sup>1</sup> where otherwise a lot of whitespace would be wasted above and/or below the line with a column vector.

Example usage:

$$\mathbf{B}_1(t) = B_1 \left( \cos(\omega_{\text{rf}}t + \varphi_{\text{rf}}), -\sin(\omega_{\text{rf}}t + \varphi_{\text{rf}}), 0 \right)^T. \quad (5.1)$$

which is even more handy for footnotes<sup>1</sup> where otherwise a lot of whitespace would be wasted above and/or below the line with a column vector.

### 5.1.3. Macros with Arguments

Sometimes you may want to be able to influence what a command does without creating a new command. For instance, if I want to stay consistent with how I denote mixtures (e.g. “pNIPAM-something mixture” vs “pNIPAM/something mixture”), I can create a macro which still needs me to tell it what the second part of the mixture is:

---

```
\newcommand{\pNIPAMbinary}[1]{\mbox{\pNIPAM/}\allowbreak#1\unskip\xspace}%
  pNIPAM in binary mixtures such as ‘‘pNIPAM/water’’
```

---

and also use the macro for any such mixture, e.g. for both [pNIPAM](#)/water and [pNIPAM](#)/ethanol.

In this example, the argument is mandatory, i.e. will complain if you don’t specify what the second part of the mixture is. You can also create commands with optional arguments (note the second set of square brackets) like

---

```
\newcommand{\TOne}[1][ ]{\ensuremath{\{T_1^{\text{trm}}\}}\xspace}%spin-lattice
  relaxation time T1
%need braces around T_1 macros to avoid ‘‘double superscript error’’ when
  writing something like \TOne^{-1}
Example usage: To then either use as \TOne without any argument or as \TOne[
  scaled] or \TOne[s, $\{17\}$0] where needed
```

---

Example usage: To then either use as  $T_1$  without any argument or as  $T_1^{\text{scaled}}$  or  $T_1^{\text{s}, 17\text{O}}$  where needed.

Yet another example in support of using macros: How much space do you allow between an equation and e.g. a comma? Say you introduce

$$\hat{\boldsymbol{\mu}} = \gamma \hat{\boldsymbol{I}} \quad , \quad (5.2)$$

---

<sup>1</sup> $\mathbf{B}_1^{\text{lin}} = 2B_1 (\cos(x), 0, 0)^T = B_1 \cdot \left[ (\cos(x), \sin(x), 0)^T + (\cos(x), -\sin(x), 0)^T \right].$

which you want to follow by “whereby  $\gamma$  is the gyromagnetic ratio”. You need to place a comma somewhere. If you like, you could keep your options open by defining a macro

---

```
\newcommand{\eqend}[1]{\text{\quad#1}}%argument is intended for
punctuation in math environment after an equation.
```

---

which currently leaves one “quad” of space and can be changed if you feel like it. You only have to consistently use it in the equations, e.g. the code for eq. (5.2) is

---

```
\begin{equation}\label{eq:magnetic_moment}
\hat{\bm{\mu}} = \gamma \hat{\bm{I}}\eqend{,}
\end{equation}
```

---

**More Complicated Macro Example** The probably most complex thing I used macros for was sample naming. For the following example, you would also need packages which handle simple calculations and allow the use of if-then-else code structure

---

```
\usepackage{calculator}%For simple calculations of e.g. automatically determine
water fraction part of sample name when etoh fraction is known. Package
suggested here https://tex.stackexchange.com/questions/453454/calculations-
on-variables-using-latex
%documentation here: https://mirrors.ibiblio.org/CTAN/macros/latex/contrib/
calculator/calculator.pdf
\usepackage{xifthen}%check if either component is 100%, and if so, suppress
label of absent component
%documentation here: https://mirror.funkfreundelandshut.de/latex/macros/latex/
contrib/xifthen/xifthen.pdf

%naming of samples with linear pNIPAM
\newcommand{\pLinSample}[2][0]{\mbox{\%mbox to prevent linebreaks in sample name
\ifthenelse{\cnttest{#2}{=}{100}}{if (outer)
{\textrm{Lin-E#2\hspace{.5em}}}%then (outer)
{\ifthenelse{\cnttest{#2}{=}{0}}{if (inner)
{\textrm{Lin-W\ensuremath{\_}\text{#1}}\SUBTRACT
{100}{#2}{\wfrac}{\wfrac}\hspace{.5em}}%then (inner)
{\textrm{Lin-E#2W\ensuremath{\_}\text{#1}}\SUBTRACT
{100}{#2}{\wfrac}{\wfrac}\hspace{.5em}}%else (inner)
}%else (outer)
}%close mbox
}%linear pNIPAM samples. Arg1=EtOH Concentration, Arg2=deviations from ‘‘0’’ (
oxygen) index for water labelling (e.g. \pLinSample[D]{0}). Syntax: \
newcommand{\commandname}[total number of arguments][default value of
optional arguments, which are numbered from 1 to the total number of
arguments]{code}
%Example usage: \pLinSample{10}, \pLinSample{100}, \pLinSample[D]{30}, \
pLinSample[D]{0}.
```

---

Example usage: Lin-E10W<sub>O</sub>90, Lin-E100, Lin-E30W<sub>D</sub>70, Lin-W<sub>D</sub>100.

## 5.2. Hyphenation

Hyphenation on linebreaks fails in some cases and this is not necessarily your fault, see <https://tex.stackexchange.com/questions/171084/why-does-usepackagebritish-babel-hyphenate-the-word-alternate-incorrectly>.

You can fix this by manually defining the hyphenation of words you notice being wrongly hyphenated in (the close to final version of) your thesis with commands like (assuming you use the british language babel package)

---

```
\babelhyphenation[british]{be-yond}
```

To check how to hyphenate a word, I sometimes used this website: <https://www.hyphenator.net/en/word/beyond>.

### 5.2.1. Controlling Linebreaks

Usually, L<sup>A</sup>T<sub>E</sub>X is good at finding good spots for linebreaks (not so good at hyphenation though, see sec. 5.2), but may be pressed for options if there are very few very long words without hyphenation options in one or in two subsequent lines.

You can avoid linebreaks by placing whatever you want to write inside an `\mbox` environment. If you overdo it and a long linebreak-protected word happens to be at the end of a line, the word will reach into the margin. Also, you can designate spots where you find it okay for L<sup>A</sup>T<sub>E</sub>X to insert a linebreak, even if it is normally hesitant to do so, via the `\allowbreak` command. I.e.

---

```
\newcommand{\pNIPAMternary}[2]{\mbox{\pNIPAM/}\allowbreak \mbox{#1\unskip/}\allowbreak #2\unskip\xspace}%pNIPAM in ternary mixtures such as ‘‘pNIPAM/ethanol/water’’
Example usages:\\
Latex Does Not Always Find A Good Spot To Place A Linebreak On Its Own \pNIPAMternary{water}{ethanol}\\%allows linebreaks in the long expression at certain places if necessary.
\newcommand{\pNIPAMbadTernary}[2]{\pNIPAM/#1/#2}%
Latex Does Not Always Find A Good Spot To Place A Linebreak On Its Own \pNIPAMbadTernary{wtr}{thnl}\\% reaches into the margin. Avoid hyphenation-triggering characters (vowels) in the arguments for demonstration purposes
Latex Does Not Always Find A Good Spot To Place A Linebreak On On Its Own \textbackslash allowbreak\\%linebreak inside the ‘‘command’’
Latex Does Not Always Find A Good Spot To Place A Linebreak On On Its Own \mbox{\textbackslash allowbreak}\\%backslash and ‘‘command’’ are forced to stay together
```

Example usages:

Latex Does Not Always Find A Good Spot To Place A Linebreak On Its Own `\pNIPAM/water/ethanol`

Latex Does Not Always Find A Good Spot To Place A Linebreak On Its Own `\pNIPAM/wtr/thnl`

## 5.2. Hyphenation

Latex Does Not Always Find A Good Spot To Place A Linebreak On On Its Own \allowbreak

Latex Does Not Always Find A Good Spot To Place A Linebreak On On Its Own  
\allowbreak

## 6. Variables

### 6.1. Booleans

Booleans are a special type of variables which can either have the value “true” or the value “false”. In L<sup>A</sup>T<sub>E</sub>X, you can setup a boolean variable like this:

---

```
\newif\ifshownotes%created a variable "shownotes" which I could then set to be
    true or false. I used this to show or hide a sections of text
\shownotesfalse% sets the value of this variable to false. change the ending
    from "false" to "true" to set it to true. I.e.: \shownotesfalse or \
    shownotesttrue
%https://tex.stackexchange.com/questions/61933/best-practice-for-getting-if-not-
    foo-conditionals
```

You can then e.g. toggle whether to show or hide a section of text by

---

```
Example usage:\\
\shownotesfalse%make sure that shownotes is false in this example
\ifshownotes%
this is a comment which is only shown if the variable ‘‘shownotes’’ has the
    value ‘‘true’’.\
\fi%end of the shownotes conditional
Here is some text which is shown regardless of the shownotes variable\xspace%
\ifshownotes%
and this is another comment which is only shown if the variable ‘‘shownotes’’
    has the value ‘‘true’’%
\fi%end of the shownotes conditional
.
```

Example usage:

Here is some text which is shown regardless of the shownotes variable.

---

```
Example usage:\\
\shownotesttrue%make sure that shownotes is true in this example
\ifshownotes%
this is a comment which is only shown if the variable ‘‘shownotes’’ has the
    value ‘‘true’’.\
\fi%end of the shownotes conditional
Here is some text which is shown regardless of the shownotes variable\xspace%
\ifshownotes%
and this is another comment which is only shown if the variable ‘‘shownotes’’
    has the value ‘‘true’’%
```



```
\fi%end of the shownotes conditional
.
```

Example usage:

this is a comment which is only shown if the variable “shownotes” has the value “true”.  
Here is some text which is shown regardless of the shownotes variable and this is another  
comment which is only shown if the variable “shownotes” has the value “true”.

### 6.1.1. Tdonotes

Using a boolean variable in this way only makes sense if it is a large section of text, or if the text needs to be adjusted in multiple places. For simple, short comments, I would recommend you use the `tdonotes` package instead. Note that I used the `parskip` package in combination with `tdonotes`, see sec. 5.1.1.

You can create notes in the margin or in between textlines with the commands

```
Example usage: \todo{text displayed in the margin} and a bit more text \todo[
  inline]{this goes into the main text area} and yet more text.
```

Example usage: and a bit more text

this goes into the main text area

text displayed  
in the margin

and yet more text.

You can also print a list of your todo notes with `\listoftodos` or hide your `tdonotes` by using the package option “disable”.

You can also set the background colour of a todo note, which I used to mark e.g. how crucial it is that I take care of it, or which proofreader made which comments. For dark colours, you will want to adjust the colour saturation so you can still read (black) text:

```
Example usage: \todo[inline, color=blue!20]{This background is blue
  with only 20 percent saturation.}
```

Example usage:

This background is blue with only 20 percent saturation.

## 6.2. Other Types of Variables

Other variables can take continuous values rather than true/false. For example, you can define a variable for the horizontal space your figures should occupy.

```
\def\defaultfigurewidth{0.95\linewidth}%used as the default value for how much
  of the linewidth a figure with a single panel should occupy
```

## 6. *Variables*

```
| \def\defaulttwosubfigwidth{0.49\linewidth}%used as the default value for how  
|      much of the linewidth a subfigure of a figure with two panels should occupy
```

## 7. Referencing Equations

You can use a subequations environment to label equations of e.g. an “align” environment as 1a, 1b, 1c etc. Each line can have a label, in case you want to refer to “eq. (1a)”. To refer to “eq. (1)”, the label needs to be placed after the start of subequations (before the align environment). For short text passages in between subequations, use `\intertext`.

---

Example usage of subequation referencing. Example code is also intended for the parent-equation referencing which is described next:

```
\begin{subequations}\label{eqs:hamiltonian_QP_EFG}
  \begin{align}
    &\hat{H}_{\text{QP}} = \frac{eQ_{\text{Moment}}}{I(2I-1)} \frac{1}{4} \left[ 3\hat{I}_z^2 - I(I+1) \right] V_{zz} \label{eq:hamiltonian_qp} \\
    &\intertext{with} \\
    &V_{zz} = \frac{eq}{2} \left[ 3\cos^2(\theta) - 1 + \eta_Q \sin^2(\theta) \cos(2\phi) \right] \label{eq:efg_lab} \quad \text{eqend{.}} \\
  \end{align}
\end{subequations}
```

Refer to a subequation by `\cref{eq:hamiltonian_qp}`, or to a number of specific subequations by `\cref{eq:hamiltonian_qp,eq:efg_lab}` without a whitespace after the comma separator of the labels

Example usage of subequation referencing. Example code is also intended for the parent-equation referencing which is described next:

$$\hat{H}_Q = \frac{eQ}{I(2I-1)} \frac{1}{4} \left[ 3\hat{I}_z^2 - I(I+1) \right] V_{zz} \quad (7.1a)$$

with

$$V_{zz} = \frac{eq}{2} \left[ 3\cos^2(\theta) - 1 + \eta_Q \sin^2(\theta) \cos(2\phi) \right] \quad (7.1b)$$

Refer to a subequation by eq. (7.1a), or to a number of specific subequations by eqs. (7.1a) and (7.1b) without a whitespace after the comma separator of the labels.

You can suppress a (sub)equation number with the “`\nonumber`” tag, i.e.

---

```
Example usage:
\begin{align}
  \overline{\expval{\hat{0}}} &= \overline{\bra{\psi}\hat{0}\ket{\psi}} \nonumber \\
\end{align}
```

## 7. Referencing Equations

$$\hat{0} = \sum_{\psi} p_{\psi} \sum_{m,n} c_{\psi,m}^* c_{\psi,n} \langle \psi_{I,m} | \hat{O} | \psi_{I,n} \rangle$$

Example usage:

$$\begin{aligned} \overline{\langle \hat{O} \rangle} &= \overline{\langle \psi | \hat{O} | \psi \rangle} \\ &= \sum_{\psi} p_{\psi} \sum_{m,n} c_{\psi,m}^* c_{\psi,n} \langle \psi_{I,m} | \hat{O} | \psi_{I,n} \rangle \quad , \end{aligned} \quad (7.2)$$

I also set up the `cleveref` package (cf sec. 2.3) such that I can use a custom command to refer to such a set as eqs. (7.1), i.e. with a plural “s” in the reference type (“eqs”) even though there is only one label in the reference command. I recommend to label sets of equations differently, i.e. `\label{eqs:hamiltonian_QP_EFG}` rather than `\label{eq:hamiltonian_QP_EFG}` (note “eqs:...” vs “eq:...”), such that it will be apparent to you from the autocomplete suggestions that there are subequations. You can of course also use this label in a standard reference command `\cref{eqs:hamiltonian_QP_EFG}`: eq. (7.1).

### 7.1. Repeating an Equation while Referring to the Original

If you want to refresh the reader’s memory of an equation which appeared a while ago or only use the result of something which is derived in detail in the appendix, you should not use a formally new equation. I think it is better to signal in the equation number that the original equation appears in a different context, which can be done with the `\tag` command:

Example usage:

```
\begin{equation*}\label{dummytag}
\correlationfunctiondef{} \eqend{.} \tag{\cref{eq:autocorrelation} (
repeated)}
\end{equation*}
Here is a reference to the appendix \cref{sec:appdx_relaxation-speddens-sto}
and an equation that is repeated from there
```

Example usage:

$$f_{2,m}(\mathcal{T}) \equiv (-1)^m \overline{R_2^{-m}(t) R_2^m(t - \mathcal{T})} \quad . \quad (\text{eq. (B.1a) (repeated)})$$

Here is a reference to an equation which is derived in the appendix: eq. (B.1).

### 7.2. Equations with Cases

Example usage:

```
\begin{subequations}\label{eq:cases}\label{eqs:qcc_anisotropy}
  \begin{align}
    &\&\text{QCC} \equiv \frac{eqe\text{QMoment}}{h} \quad \text{\label{eq:qcc}} \\
    &\intertext{and} \\
    &\&\text{QCC} \equiv \delta_Q \frac{4I(2I-1)}{3(2k-1)} \quad \text{\eqend{where }k=} \\
    &\begin{cases}
      1 & \text{\text{for } $^2$H} \\
      3/2 & \text{\text{for } $^{17}$O}
    \end{cases} \\
    &\text{Not sure about fully general validity though} \\
    &\text{integer spin. Not sure about fully general validity though} \\
    &\end{cases} \quad \text{\label{eq:anisotropy}\eqend{.}} \\
  \end{align}
\end{subequations}
```

Example usage:

$$C_Q \equiv \frac{eqeQ}{h} \quad (7.3a)$$

and

$$C_Q \equiv \delta_Q \frac{4I(2I-1)}{3(2k-1)} \quad \text{where } k = \begin{cases} 1 & \text{for } ^2\text{H} \\ 3/2 & \text{for } ^{17}\text{O} \end{cases} \quad (7.3b)$$

### 7.3. Multiline Equation

For long mathematical expressions you will need to have a linebreak somewhere. With the multiline environment, you can place the linebreak of an equation like eq. (7.4) where it does not disrupt the mathematics too much, or maybe even helps compare expressions:

```
Example usage:
\begin{multiline}\label{eq:diff_two-step-decay}
  S(t_{\mathrm{m}}) = \left[ A_{\mathrm{w}} \exp(- \left( \gamma_{\mathrm{H}} \right. \right. \\
\mathrm{G} t_{\mathrm{e}} \left. \right)^2 D_{\mathrm{w}} \left( \frac{2}{3} t_{\mathrm{m}} \right. \\
\left. \left. + t_{\mathrm{m}} \right) \right] + \text{\right.} \quad \text{\%need to close/open \left\right pair} \\
\text{on linebreak. use vphantom{highest expression} to match sizes} \\
\left. A_{\mathrm{p}} \exp(- \left( \gamma_{\mathrm{H}} \right. \right. \mathrm{G} t_{\mathrm{e}} \left. \right)^2 D_{\mathrm{p}} \left( \frac{2}{3} t_{\mathrm{e}} + t_{\mathrm{m}} \right. \\
\left. \left. \right) \right] \text{\vphantom{\exp(\frac{2}{3})}} \text{\right} \\
* \exp(- \left( \frac{2t_{\mathrm{e}} + t_{\mathrm{m}}}{T_0} \right) \\
\text{\beta}) \quad \text{\eqend{.}} \\
\end{multiline}
```

## 7. Referencing Equations

Example usage:

$$S(t_{\text{m}}) = \left[ A_{\text{w}} \exp\left(-(\gamma_{\text{1H}} G t_{\text{e}})^2 D_{\text{w}} \left(\frac{2}{3} t_{\text{e}} + t_{\text{m}}\right)\right) + \right. \\ \left. A_{\text{p}} \exp\left(-(\gamma_{\text{1H}} G t_{\text{e}})^2 D_{\text{p}} \left(\frac{2}{3} t_{\text{e}} + t_{\text{m}}\right)\right) \right] * \exp\left(-\left(\frac{2t_{\text{e}} + t_{\text{m}}}{T_1}\right)^\beta\right) \quad . \quad (7.4)$$

I suppose using multiline for this is cleaner than suppressing the equation number as in eq. (7.2).

## 8. Figures

### 8.1. Placement

Have a simple figure, fig. 8.1.

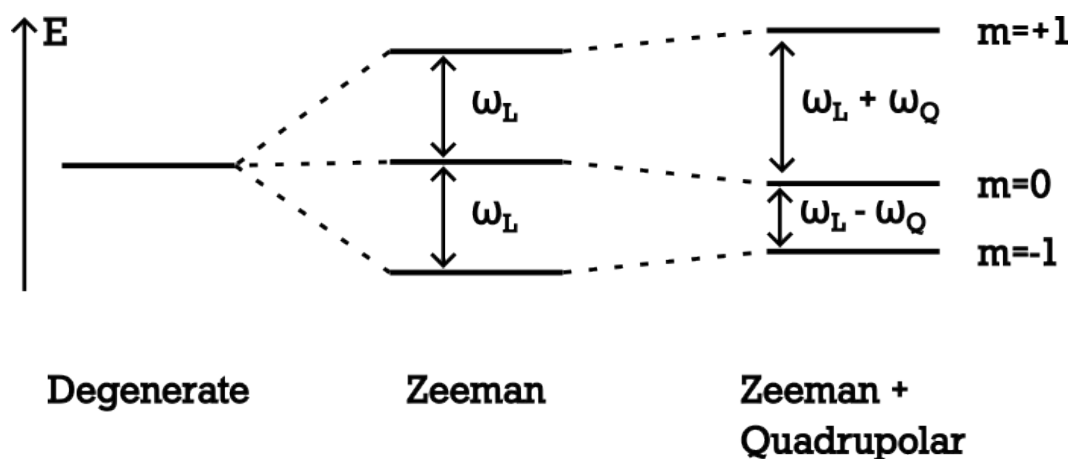
To avoid wasting (horizontal) space with small figures, you can find two small figures and place them side by side. Alignment is easier if you surround the figures with a minipage, cf fig. 8.3.

---

```
Example usage: \cref{fig:binodal-spinodal-phase-diagram}
\begin{figure}
  \centering
  \begin{minipage}[t]{0.4\textwidth}
    \centering
    \includegraphics[width=\linewidth]{Figures/
    FloryHugginsLattice_GeddeEtAl_Springer2019}
    \captionof{figure}{Distribution of a polymer and a low
    molecular mass solvent on a (2-dimensional) lattice as per the Flory-
    Huggins theory. Figure reproduced from \autocite{Gedde2019}.}
    \label{fig:floryhugginslattice}
  \end{minipage}\hfill%
  \begin{minipage}[t]{0.55\textwidth}
    \centering
    \includegraphics[width=\linewidth]{Figures/
    PhaseDiagram_LCST_Rubinstein_OxfordUnivPress2004}
    \captionof{figure}{Top: (Scaled) change in free energy due to
    mixing for a symmetric mixture. The minima are marked as  $\phi^{\prime}$  and
     $\phi^{\prime\prime}$  and the inflection points as  $\phi_{\mathrm{sp1}}$  and
     $\phi_{\mathrm{sp2}}$ . Bottom: Phase diagram of the mixture. The thick dashed
    and solid lines represent the spinodal and binodal, respectively. From the
    top panel, values of the binodal (minima) and spinodal (inflection points)
    at a given value of  $N\chi$  can be derived. Figure reproduced from \
    autocite{Rubinstein2004}.}
    \label{fig:binodal-spinodal-phase-diagram}
  \end{minipage}
\end{figure}
```

Example usage: fig. 8.3.

To give you another idea: mosaic plots offer some more advanced placement options for, e.g. a large panel on the left and two smaller panels on the right with the (combined) same height. I, however, ended up creating such a plot with python and – as far as L<sup>A</sup>T<sub>E</sub>X



**Figure 8.1.:** Sketch of the shift in terms of angular frequency of initially degenerate energy levels of a spin  $I = 1$  nucleus due to Zeeman and quadrupolar interaction (first order, not to scale).

is concerned – include it as a single image.

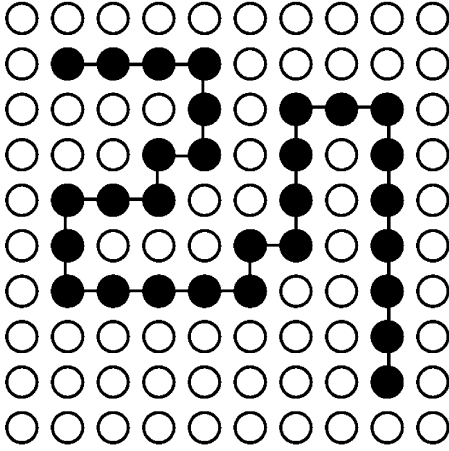
Alternatively, wrapping text around a figure could be desired. If so, see commented lines in the source code.

## 8.2. Subplot Labelling

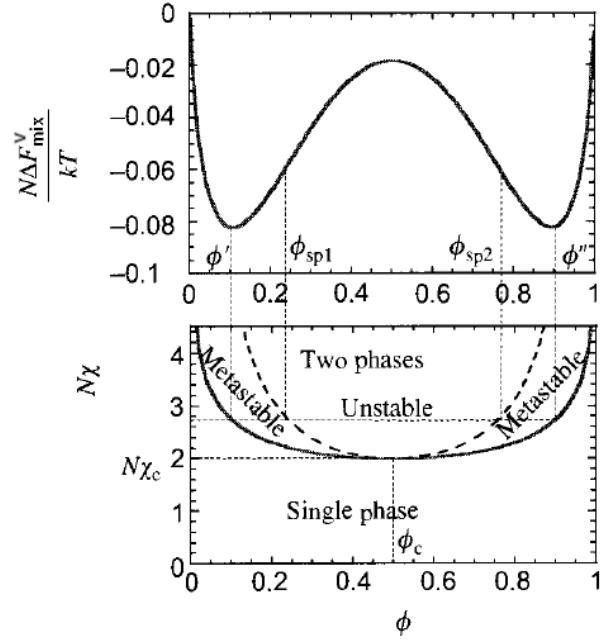
Here is a figure fig. 8.4 with a faked second subfigure (`width=0`, `\phantomcaption`, `\label`) in order to simulate the desired subplot labelling. This is useful if the image you want to show already contains the labels in the panels and you don't want a caption to repeat it and/or use up space.

```
\begin{figure}
  \begin{subfigure}{\defaultfigurewidth}
    \centering
    \includegraphics[width=\linewidth]{Figures/Complete_Figure.png}
    \phantomcaption
    \label{fig:label_for_first_subfigure}
  \end{subfigure}%\hfil
  \begin{subfigure}{0\linewidth}
    \phantomcaption
    \label{fig:label_for_second_subfigure}
  \end{subfigure}
  \caption{Caption for complete figure.}
  \label{fig:label_for_complete_figure}
\end{figure}
```

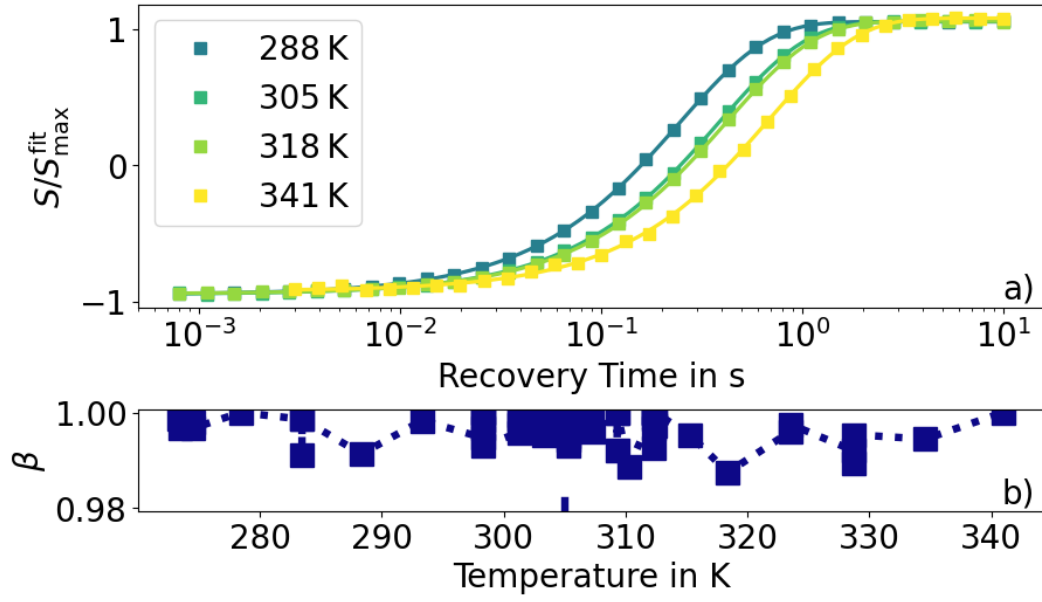




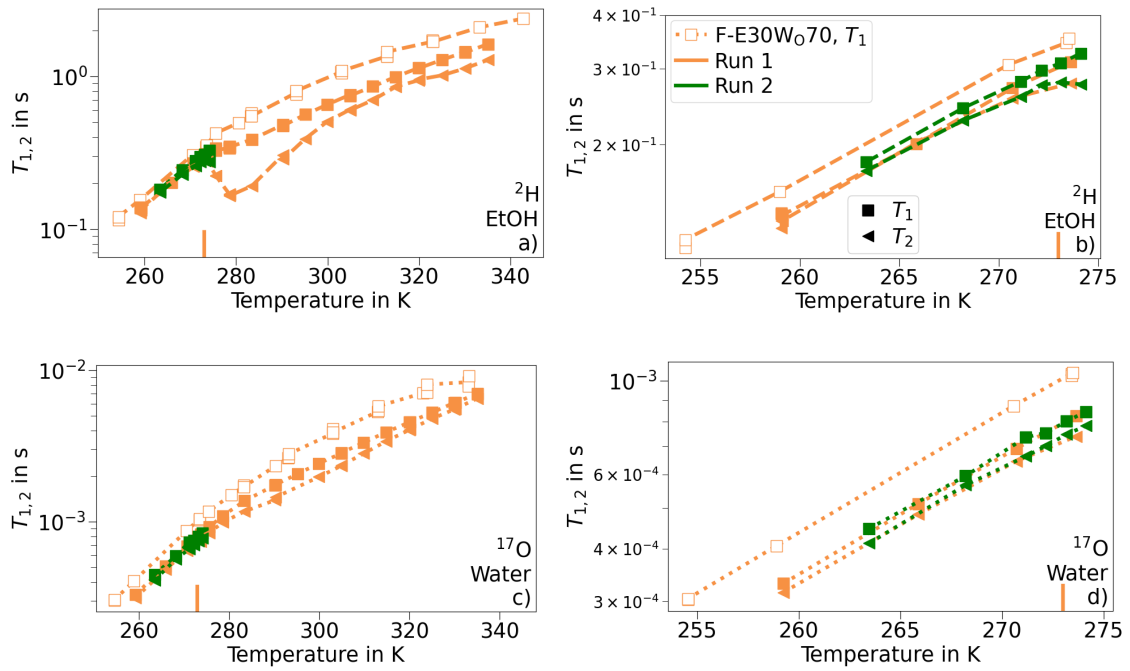
**Figure 8.2.:** Distribution of a polymer and a low molecular mass solvent on a (2-dimensional) lattice as per the Flory-Huggins theory. Figure reproduced from [GH19].



**Figure 8.3.:** Top: (Scaled) change in free energy due to mixing for a symmetric mixture. The minima are marked as  $\phi'$  and  $\phi''$  and the inflection points as  $\phi_{sp1}$  and  $\phi_{sp2}$ . Bottom: Phase diagram of the mixture. The thick dashed and solid lines represent the spinodal and binodal, respectively. From the top panel, values of the binodal (minima) and spinodal (inflection points) at a given value of  $N\chi$  can be derived. Figure reproduced from [RC04].



**Figure 8.4.:** Normalized build-up of  $^2\text{H}$  magnetization from inversion-recovery experiments at  $\omega_L/(2\pi) \approx 46$  MHz for various temperatures, together with fits with a stretched exponential function **a)**. Resulting stretching parameters  $\beta$  are shown in a narrow range in **b)**, the vertical line in **b)** at 305 K marks the *demixing temperature* for pNIPAM in water [CF02; Bis+14].

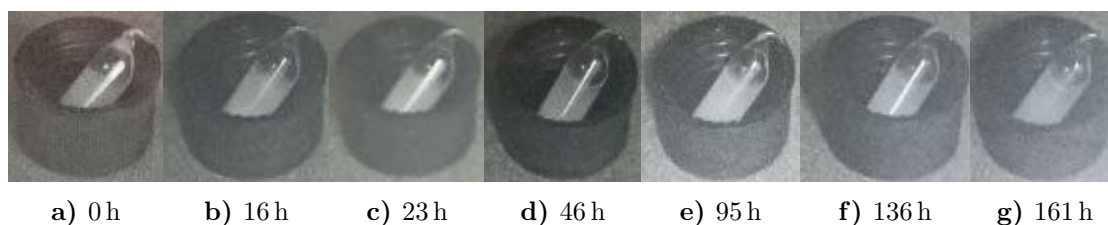


**Figure 8.5.:**  $^2\text{H}$  a), b) and  $^{17}\text{O}$  c), d) relaxation times of Lin-E30W<sub>070</sub> from the original (Run 1) and a repeat (Run 2) series of measurements to test reproducibility. The scales on the ordinates of a) and c) capture the variation of the relaxation times across all of the investigated temperatures, while b) and d) provide magnified views on the region up to the demixing temperature. Relaxation times of F-E30W<sub>070</sub> are shown for reference. The vertical line marks the demixing temperature. The data in this figure has been published in the supplementary information to [Sä+25].

### 8.3. Cropping

Here are two multi-subfigure figures with special layout figs. 8.5 and 8.6. Subfigure vertical alignment for different aspect ratios is cumbersome. You can either write many lines of code, or you can obtain the image heights the figure requests by looking at the log file of an initial compile run, where no fixed heights are set, and then manually set the heights of the subfigures (in combination with the `keepaspectratio` option) to an appropriate value (cf <https://tex.stackexchange.com/questions/389797/fill-textwidth-with-equally-height-subfigures-of-different-aspect-ratios>). You will need to have a look in the log file for this, but opening the log with a text editor of your choice and a simple keyword search for the filename will point you to the right place.

## 8. Figures



**Figure 8.6.:** Photographs of a solution of linear **pNIPAM** (10 wt%) in  $D_2O$  taken at the indicated times through the glass pane of an oven maintaining a temperature of  $\sim 40^\circ C$  for several days.

## 9. Table and Sample Macros

Here is a table, table [9.1](#), where some cells are joined with the `\multirow` command. Also, the sample-name macros (see sec. [5.1.3](#)) are used.

## 9. Table and Sample Macros

Shorthand(s)	EtOH Water	Labelling	Mention in Publication
Lin-W <sub>D</sub> 100	- 100 vol%	<sup>2</sup> H <sub>2</sub> O	[Sä+24]
Lin-W <sub>O</sub> 100, F-W <sub>O</sub> 100	- 100 vol%	H <sub>2</sub> <sup>17</sup> O	[Sä+24] (SI), [Sä+25]
Lin-E10W <sub>O</sub> 90, F-E10W <sub>O</sub> 90	90 vol% 10 vol%	CH <sub>3</sub> C <sup>2</sup> H <sub>2</sub> OH, H <sub>2</sub> <sup>17</sup> O	[Sä+25]
Lin-E20W <sub>O</sub> 80, F-E20W <sub>O</sub> 80	80 vol% 20 vol%	CH <sub>3</sub> C <sup>2</sup> H <sub>2</sub> OH, H <sub>2</sub> <sup>17</sup> O	[Sä+25]
Lin-E30W <sub>D</sub> 70, F-E30W <sub>D</sub> 70	30 vol% 70 vol%	CH <sub>3</sub> CH <sub>2</sub> OH, <sup>2</sup> H <sub>2</sub> O	[Sä+25]
Lin-E30W <sub>O</sub> 70, F-E30W <sub>O</sub> 70	30 vol% 70 vol%	CH <sub>3</sub> C <sup>2</sup> H <sub>2</sub> OH, H <sub>2</sub> <sup>17</sup> O	[Sä+25]
Lin-E40W <sub>O</sub> 60, F-E40W <sub>O</sub> 60	40 vol% 60 vol%	CH <sub>3</sub> C <sup>2</sup> H <sub>2</sub> OH, H <sub>2</sub> <sup>17</sup> O	[Sä+25]
Lin-E50W <sub>O</sub> 50, F-E50W <sub>O</sub> 50	50 vol% 50 vol%	CH <sub>3</sub> C <sup>2</sup> H <sub>2</sub> OH, H <sub>2</sub> <sup>17</sup> O	[Sä+25]
Lin-E60W <sub>O</sub> 40, F-E60W <sub>O</sub> 40	60 vol% 40 vol%	CH <sub>3</sub> C <sup>2</sup> H <sub>2</sub> OH, H <sub>2</sub> <sup>17</sup> O	[Sä+25]
Lin-E70W <sub>O</sub> 30, F-E70W <sub>O</sub> 30	70 vol% 30 vol%	CH <sub>3</sub> C <sup>2</sup> H <sub>2</sub> OH, H <sub>2</sub> <sup>17</sup> O	[Sä+25]
Lin-E90W <sub>O</sub> 10, F-E90W <sub>O</sub> 10	90 vol% 10 vol%	CH <sub>3</sub> C <sup>2</sup> H <sub>2</sub> OH, H <sub>2</sub> <sup>17</sup> O	[Sä+25]
Lin-E100, F-E100	100 vol% -	CH <sub>3</sub> C <sup>2</sup> H <sub>2</sub> OH, -	[Sä+25]
MG-W <sub>D</sub> 100	- 100 vol%	<sup>2</sup> H <sub>2</sub> O	-
Lin*-W <sub>D</sub> 100	- 100 vol%	<sup>2</sup> H <sub>2</sub> O	[Sä+24], SI
Lin*-E30W <sub>O</sub> 70	30 vol% 100 vol%	CH <sub>3</sub> C <sup>2</sup> H <sub>2</sub> OH, <sup>2</sup> H <sub>2</sub> O	-

**Table 9.1.:** List of samples, introducing abbreviations and corresponding solvent concentrations and labelling. Abbreviations denote polymer type (**L**inear, **M**icro**G**el, polymer-**F**ree), **E**thanol and **W**ater concentrations (in vol%) and a subscript to indicate which isotope labelling was used for the water component. Thereby the shorthand notation also implicitly gives the labelling of ethanol (W<sub>O</sub> → ethanol-d<sub>2</sub>, W<sub>D</sub> → natural abundance ethanol). Samples prepared for experiments in the 1 GHz-AEON spectrometer are marked with a star, e.g. Lin\*-W<sub>D</sub>100. All polymer samples listed here contain 4 wt% polymer. Note that for neat D<sub>2</sub>O, data from literature [Hin+71] was used. Note further that hydrogen exchange leads to a distribution of <sup>2</sup>H between water and ethanol in samples such as F-E30W<sub>D</sub>70, whereby it is to be expected that  $\gtrsim 90\%$  of <sup>2</sup>H is located in water molecules.

## Part II. Conclusion

In the conclusion, I want to reintroduce acronyms as if they had not been mentioned before, see sec. 4.1. This way, since some readers may read only the conclusion, they don't have to look through the glossary to find out what the acronym stands for. However, as for any mention of acronyms in the document, if there is only one document-wide use of some acronym that happens to be placed in the conclusion (maybe in a paragraph about future projects / outlook), the term should be spelled out without introducing its abbreviation. This makes complete glossary resets a bad idea and makes a completely automatized solution very tricky, although not impossible. As a compromise, I manually used the `\fakefirstacr` macro for every conclusion-first occurrence of an acronym.

I mention *poly(N-isopropylacrylamide)* (pNIPAM) twice pNIPAM, as an example for an often-used acronym. I mention what a *athermal* state is to check proper function of the non-acronym glossary and also use the test case from before (see sec. 4.1.1), *test multiple-use single in conclusion* (TMUSC), and another test case now: test single-use in conclusion. If you care about acronym formatting depending on their occurrence count (e.g. more than one occurrence), don't forget to also check the single-use test acronym in sec. 4.1.

# Part III. Appendix

## A. Including the Appendix in your Main File

Before you start the appendix, either by writing directly in your document or by inserting a separate .tex file, you should use the `\appendix` command, cf. main file of this template.

---

```
\appendix%signals some commonly reasonable changes, e.g. a change in chapter
      numbering from arabic to alphabetic
\input{Diss_Appendix.tex}%information which is nice to have, but not essential
      to follow the arguments in the main text
```

---

## B. Reusing (Parts of) an Equation

Equations (B.1) make use of macros which print a given math expression, such that I can derive this expression in the appendix and use the exact same expression (including potential future changes) in the main text. To help you jump back and forth in this template, have this poorly formatted (you are not supposed to reference the repeat equation anyway) link: [eq. \(B.1a\) \(repeated\)](#).

$$f_{2,m}(\mathcal{T}) \equiv (-1)^m \overline{R_2^{-m}(t) R_2^m(t - \mathcal{T})} \quad (\text{B.1a})$$

and its half-sided Fourier transform

$$\tilde{J}_{2,m}(\omega) \equiv \int_0^\infty f_{2,m}(\mathcal{T}) \exp(im\omega) d\mathcal{T} \quad \text{where } \omega = -\gamma B_0 \quad . \quad (\text{B.1b})$$



# Acknowledgements

No new L<sup>A</sup>T<sub>E</sub>X tricks.

# Abbreviations

**CPMG** Carr-Purcell-Meiboom-Gill. [10–12](#)

**LCST** lower critical solution temperature. [13](#), [14](#)

**pNIPAM** poly(N-isopropylacrylamide). [12](#), [21](#), [24](#), [35](#), [37](#), [40](#)

**TMUSC** test multiple-use single in conclusion. [15](#), [40](#)

# Bibliography

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