Universität Zürich[UZH]

Department of Chemistry

Handbook on Writing Laboratory Reports

Georg Artus, Stefan Bienz, Koushik Venkatesan, Jan Helbing

We thank our colleagues Jürg Hutter, Bernhard Spingler, Sergio Gloor, and the students Manuela Zimmermann and Sebastian Wellig for discussion and ideas. We thank Phil Johnson for editing the English language of version 1.00.

Version 1.21, August 2020

Table of Contents

1 Introduction 5
2 General Guidelines 5
2.1 Purpose of a Report 5
2.2 Good Scientific Practice 6
2.2.1 General Ideas 6
2.2.2 Why, When, and What to Cite? 6
2.3 How to Tackle a Report 8
2.3.1 Starting a Report 8
2.3.2 Finalising a Report 9
3 Structure of a Scientific Report 9
3.1 Title and Title Page 10
3.2 Table of contents 10
3.3 Abstract / Summary 10
3.4 Introduction 11
3.5 Results and Discussion 11
3.6 Conclusion 12
3.7 Experimental Section 12
3.8 References 15
3.9 Appendices 15
4 Style Guide 15
4.1 Physical Quantities and Units 15
4.2 Tables 17
4.3 Schemes and Figures 19
4.3.1 General Considerations 19
4.3.2 Schemes 20
4.3.3 Figures 20
4.4 Analytical Data 23
4.4.1 Appearance 23
4.4.2 Purity 23
4.4.3 Chromatography 24
4.4.4 Refractive Index, Boiling Point, and Melting Point 24
4.4.5 Specific Rotation 24
4.4.6 UV-Vis Spectra 25
4.4.7 IR Spectra 25
4.4.8 ^{1}H-NMR Spectra 25
4.4.9 ^{13}C-NMR Spectra 26
4.4.10 MS Spectra 26
4.4.11 Magnetic Susceptibility 27
4.4.12 Elemental Analysis 27
4.5 References and Citations 28
4.5.1 Types of Quotations 28
4.5.2 Technical Aspects of Citing 28
4.6 Text 31
4.6.1 Active or Passive Voice 31
4.6.2 Tense 31
4.6.3 Writing Style 32
4.6.4 Fonts 33
5 Efficient Use of a Word Processor 34
5.1 Automatic Numbering 34
5.1.1 Cross-References 34

5.1.2 Automatically Generated Lists 35
5.1.3 Footnotes 35
5.2 Style Sheets 35
5.3 Search and Replace 35
5.4 Auto-Correct or Auto-Replace 35
5.5 Shortcuts and Macros 36
6 References 36

1 Introduction

Writing plays a very important role in science. The most brilliant discovery in a laboratory is useless unless the knowledge about it disseminates to be used and developed by other scientists. The most important way of transmitting scientific findings are written publications: articles in journals, books, or academic theses. These publications determine the reputation and qualification of a scientist. Hence, after maybe years of hard work in the laboratory, you would like to present the results of your work as well as possible to your colleagues in the field. Clearly, the presentation of scientific results requires adequate writing skills.

Scientific writing is also an indispensable part of learning. Writing a scientific text or a laboratory report forces you to think about what you have done and why. Writing helps you to uncover (and then of course fill) gaps in your knowledge or understanding. Any discussion of scientific text with your colleagues or your supervisor is very instructive. The list of connections between writing and scientific understanding is much longer than these few examples. In short, writing helps you to advance in science.

Furthermore, writing is one of the most important communication skills in general, not only in science. Also in industry, management, or administration, written documents are the basis of internal and external communication. Thus, any investment in your writing skills will benefit you in the future.

This handbook guides you through the first steps of scientific writing. It focusses mainly on the formalism and the technical aspects of how to write a report. This handbook can just touch on an attractive writing style, which will become more important in a later stage of your studies. For your very first laboratory reports, you will not have to follow all of the instructions provided in this guide at once. Rather, the requirements will increase over time. Please refer to the documents of the specific laboratory course for more detailed instructions. Learning how to write is largely learning by doing. It needs time, practice, and feedback. Publishing your first article in a scientific journal will reward you for many years of training!

2 General Guidelines

2.1 Purpose of a Report

The research or laboratory report is a document with which you present your results to a selected audience. Your first readers are the teaching assistants in your laboratory course. Later, the audience is your supervisors and finally the scientific community in your field.

The practical purpose of a report is to summarize your results in a comprehensive way. Other chemists should understand what you did, why, and how you did it. They should learn something from your results. The most brilliant ideas and most clever experiments are non-existent if unpublished, or maybe even worse, published in an incomprehensible and doubtful manner. Therefore, you must present the experiments and results in a form that is adequate and digestible for the readers. The description of your devices and experimental procedures has to be exact and sufficiently detailed such that other chemists are able to reproduce your experiments. The experiments have to be put into a context, they have to be discussed, interpreted, and all relevant information that support your interpretations must be included. Learning how to *report scientific experiments meticulously and comprehensibly* is the main purpose of undergraduate laboratory reports.

Presenting specific results by means of a report is only one part of the story. It is equally important is that you present yourself, your effort, your abilities, and your knowledge to your colleagues, your teaching assistant, to your supervisor, and later to the scientific community. This is an important contribution to your reputation. Other scientists are rarely able to judge your work in the laboratory directly. They assess your abilities and expertise by what they read about your work! Although the scientific results should be most important in a report, the idea of presenting ones work most effectively is receiving more and more attention.

2.2 Good Scientific Practice

2.2.1 General Ideas

The fundamentals of good scientific practice are integrity and honesty. Trust and respect are the rewards for honesty. Dishonesty destroys the trust in you, in your institution, and in your discipline. Of course, this is all the more valid for writing reports. Experiments with unclear results are frequent. Only whether and how you publish such results distinguishes between fraud and honesty.

Falsification or fabrication of data are extreme cases of scientific misconduct. In addition, reporting only the data that support your hypothesis but disregarding contradictory data is dishonest. Extreme offences against good scientific practice are punished by depriving academic titles. Scientific misconduct in a laboratory course can lead to the expulsion from that course. We recommend to consult the guidelines of the University of Zurich and further literature on scientific misconduct.[1–4]

Consider the following guidelines for writing laboratory reports or publications:

- Be honest with yourself and your readers.
- Never write something you do not understand. If you do not understand something, it might indeed be wrong!
- Be open to your own doubts and doubts expressed by others.
- Good scientific practice means accuracy, clarity, unambiguity, and reproducibility. These general ideas serve as guidelines when you have to report data or experiments where no example or author guideline is available.
- Separate facts from interpretation or even speculation (*cf.* section 4.6).
- A report can only be as good as the experiments it is based on. Therefore, good reports require well-designed experiments and properly conducted experimental work. Of course, complete and sound notes in your laboratory book are a must!
- Recognize and acknowledge the contributions of others in a fair way (see section 4.5). Since citations are an important and sensitive matter, we dedicate the section 2.2.2 to this topic.

2.2.2 Why, When, and What to Cite?

One basic answer to the question in the title of this section is citing is a matter of honesty and respect. Planning, performing, and publishing good science is difficult and demanding. Such work deserves respect! Citations express this respect. Any citation of your work indicates that your efforts have an effect and are of value to others. Being cited is satisfying. This reward is one of the motivations to perform research. Therefore, show respect for the work of others and cite them in a fair way, just as you wish to be cited by others.

Reproducing, using, or copying data, text, ideas or artwork from other sources without proper citation (and thereby pretending it is your work) is plagiarism and a serious form of scientific misconduct. Such behaviour is detrimental to science and to your reputation. Note that laboratory reports may be checked by professional plagiarism detection tools in case of a clear suspicion or on a spot check basis.

More specific reasons for citing the work of others are:[5]

- To refer to known procedures, measurements, techniques, or theories instead of describing these in detail. There is no need to reproduce what can be found in the literature unless this detailed information is necessary for the reader to understand your text.
- To mention other work which confirms or contradicts your results.
- To acknowledge similar work.
- To acknowledge the ideas or work of others which you have used for your report.
- To honour pioneers of a specific field.
- To inform the reader about further literature of interest.

Cite only work you have read yourself. Cite only work you understand. Do not cite the work of others just because your colleagues did so. Use and cite only sources which are available and thus verifiable. Good sources are books, articles in scientific journals, patents, or academic theses. Internal or even confidential reports, personal communications, or other unofficial sources are problematic. Cite scientific sources. These sources were written by scientists. Ideally, they were also reviewed and edited by experts in the field.

Sources from the internet require special attention. Webpages may change or even disappear very quickly. In addition, the necessary data for an unambiguous citation (author names, title of a document, version number, publisher, or institution, date of publishing, date of access) are often far from clear. These facts contradict scientific principles. However, the number of scientifically valuable online sources is increasing constantly. Therefore, banning online sources is also inappropriate. The general scientific standards—which kind of online source is acceptable as scientific source and how it has to be cited (*cf.* section 4.5.2)—are lagging far behind the fast development of internet technology. You may use and cite online databases, electronic versions of text books, or other data which is also available in a printed edition.[6] Trustworthy sources can be identified by the existence and easy accessibility of the bibliographic data listed above in brackets and by the fact that the webpage itself cites scientific sources as origin of the data the webpage presents.[7] We do not accept dubious internet sources in laboratory reports.

Undoubtedly, Wikipedia is a powerful and easily accessible database of common knowledge. The quality of articles is improving constantly.[8] However, there is no common agreement whether Wikipedia is an acceptable scientific source or not.[9] Consequently, citations referring to Wikipedia are very rare in the scientific literature. Therefore, we recommend that you preferentially use chemical literature, chemical databases, and chemical textbooks. Be aware that your reader may interpret any citation of Wikipedia as unscientific style. Using Wikipedia without citing it would be scientific misconduct.

Much more important than the kind of source is that you critically evaluate the data provided by this source. Are the values you want to cite reliable? Are there experimental ambiguities? Does contradictory data exist in the literature or did other authors question the results? Are the conditions, which were used in the literature, truly comparable to your experiment? If only questionable sources are available, discuss potential problems and ambiguities along with the cited data in your report. Accepting data blindly from the literature is bad scientific practice.

One of the basic principles of science, namely that science is self-correcting, is based on the critical assessment and re-assessment of already published results!

Citing in publications is more complex than in laboratory reports. Some reasons for this may be a maximum number of allowed citations for articles in journals, limited access to literature, language issues, and that citations are used (or also abused) as a means to assess the quality of an author (*h*-index), a group, a scientific journal (journal impact factor), an institution, or even whole universities (university rankings). More information on this topic can be found in the literature.[5,10]

2.3 How to Tackle a Report

2.3.1 Starting a Report

To many people (including scientists), the idea of sitting in front of a blank sheet of paper and having to write something is dreadful. Start with your report only after having finished all of the necessary evaluation of data. Separate the work in small and digestible portions.

It is a very good idea not to start writing in full sentences. Instead, concentrate on the outline of your report first. To complete an outline, start with a template that contains only the main headlines (abstract, introduction, experimental part …). Collect all ideas what to write as keywords in the appropriate section. Use the outline view of your word processor to collect, group and rearrange the keywords easily. Use different levels to organise your keywords. You may use keywords instead of figures at this stage.

Start with the experimental section because you can transfer this part from your laboratory notebook easily (the keywords may be: list of materials and devices, make solutions, table with concentrations, measured absorption values …). In addition, consult the instructions to the experiment as a reminder. What are the specific tasks to perform or the questions to answer? (Keywords may be: graph with all spectra, *Arrhenius* plot, derive equilibrium constants, calculate yield)

Check whether all your keywords are in the correct section (*cf.* chapter 3).

Check and correct the order of your keywords for a logical sequence. Do you present all the experiments in a meaningful sequence? Do you present the analysis of your data before you derive the results? Are all necessary data provided to support the conclusion? Do you interpret the results after presenting the results? Do you present data from the literature at the right place? Do you know how to link one idea to the next one? Do you use the figures where the reader needs them? Arranging your keywords in correct order is a very important step because the resulting sequence of ideas determines the “story line” or “plot” of your final report. Without a well-planned thread, your final report will be chaotic and badly composed.

It is customary to use more than one numbered section per chapter or more than one numbered subsection per section. If this is not the case, rearrange your sections or the numbering level of single numbered sections.

Next, you may want to design your figures. Start with a hand drawn sketch until the figure fulfils your needs. Finalising the figure on the computer can wait until the outline of your report is truly fixed.

If your list of keywords is complete and ordered you have managed to finish an important part of your report! Only now, you should start writing in full sentences. It is much easier to write a paragraph based on a finished outline because starting points and end points for each paragraph are given by the preceding and the subsequent keyword in your outline. Write the introduction and the abstract last.

2.3.2 Finalising a Report

Every draft needs to be revised, amended, and edited several times. Read your text slowly and ask yourself: Do you understand your text? Are the sentences short, simple, straightforward, and grammatically correct? Do they make sense? Are they linked? Do you find empty phrases or verbs in the wrong tense?

Use the spell-checker and the grammar-correcting tool of your word processing software. These tools are not always reliable but may indicate words or phrases that may need editing.

Read and check the final report *in printed form*! If you want to submit your report in the portable document format (PDF), check the *printed PDF-file* and not the printout from your word processor. Is everything legible, especially small lettering in figures? Is all formatting correct and consistent? Are cross-references updated and correct? Are all special characters and symbols as they should be? Are graphics and tables positioned close to their first callout? Is there white space because of unfavourable page breaks?

It is a good idea to ask a knowledgeable person to review your report before you hand it in. You will be surprised how valuable (and often unexpected) the comments of a peer can be.

3 Structure of a Scientific Report

A report consists of two major parts. In the experimental part, also known as "materials and methods", you present the hard facts: the procedures, equipment and materials you used, and the raw data you obtained from your experiments. In the remaining part of the report—often termed theoretical part—you elaborate on the investigation, interpret the experimental facts and discuss the results in a wider context, including the literature. This comprises the sections introduction, results, discussion, and conclusion. It may be appropriate to combine results and discussion into one section. Finally, all references to existing literature are listed at the end. (A publication or academic thesis may contain additional sections for acknowledgements or author information, a table of contents, list of abbreviations or figures, or supporting information. The latter is considered to be part of a publication but is available only online.) The structures of the theoretical and experimental parts are standardised and allow solely small variations.

Contrary to this, style, formatting and layout of a report are more flexible. Often, there is no clear borderline between right and wrong with regard to style, formatting, or notation. In addition, different habits are common in different fields of science.

However, this freedom in terms of style and formatting may cause problems. For beginners, it is difficult to judge which style or notation to use, *e.g.* for the presentation of an error range or how to correctly format NMR-data. Therefore, we define in this handbook the standards that you will have to follow in all of our laboratory courses. These strict and clear rules have several advantages:

- They prevent you from wasting time on formal issues.
- They force you to use formats and notations consistently. Inconsistent formatting within one and the same report (*cf.* the table heads in Table **Fehler! Verweisquelle konnte nicht gefunden werden.** in section 4.2 as an example) may raise the justifiable question whether you are working similarly inconsistently and unreliably in the laboratory!

- Strict rules are common in scientific publishing. Any manuscript, which is submitted to a scientific journal, has to be formatted according to the specific (and often very strict) rules of the specific journal.
  Very often, several individual reports or parts of reports have to be compiled to one manuscript. This is the case when several researchers, who work on a common project, combine their results to a single publication or when several partial reports of one and the same researcher have to be combined to an academic thesis. Adapting different styles of individual documents is very laborious and time-consuming (think of fonts, font sizes, citation formats, line styles in plots, layout of tables, presentation of analytical data, different settings in *ChemDraw*, and so on).
- Uniform and fair grading of the reports is difficult without clear rules.

3.1 Title and Title Page

The title of a report or a publication should be short and descriptive, giving concise information on the topic and possibly also on the result of the investigation. Avoid using less common abbreviations, long IUPAC names, or excessive jargon.

For laboratory reports, depending on the specific course, further information such as bench number, project/program number, experiment number, the date when the experiment was done, and the name of the responsible teaching assistant has to be provided as well. Finally, the date of completion of the report is added.

For publications, the title is given on the title page followed by the name(s) of the author(s), their affiliation(s), their contact data, and a list of keywords.

3.2 Table of contents

Add a table of contents if your report is long or contains many chapters or sections.
Tables of figures, schemes, equations, or any other items only make sense for longer reports with many such numbered items.

3.3 Abstract / Summary

The abstract summarizes the most important points of your report. This may comprise one introductory sentence, a short description of the reaction you conducted, specific methods you may have used, and, of course the main results. If you used standard techniques, that are well known in chemistry or that are even named after scientists, mention these by their name, *e.g.* "*Ugi* four-component reaction" or "Evaluation of the data according to the *Stern–Volmer* equation ..."

The abstract should be comprehensible in itself. It should not require the reader to consult the main text. Abbreviations and citations are not used. The overall length of an abstract for a laboratory report roughly ranges from a few lines to half a page. Scientific journals often limit the length of an abstract, *e.g.* to 150 words.

Writing an abstract is a very good training for extracting the most important points out of a scientific report. Differentiating important things from less important ones sounds simple but it is not! Summarising your work in an abstract requires that all other parts are already written. Therefore, write the abstract last.

3.4 Introduction

Imagine the reader of your report is educated in the field but does not have explicit knowledge about the experiment you are reporting. The task of the introduction is to introduce the particular aspects of your chemistry and prepare the reader to understand your report. Therefore, the introduction should describe the problem you worked on in a wider chemical context. This may be, for example, a summary of the current literature, previous but contradictory findings, a historical review of the phenomenon under scrutiny, the relevance of a chemical reaction, or the application of the compound that you synthesized. Based on that, describe the specific question you want to answer with your work and why this question is of relevance. The last sentence may give a brief but general outlook to what you did and which methods you applied. The introduction does not contain detailed information on the experiments or the results!

In case you use specific technical terms in your report repeatedly, you may abbreviate them. Upon the first occurrence of the term that you want to abbreviate, mention the complete term followed by your abbreviation in brackets. For example: “The applied technique was scanning transmission electron microscopy (STEM).” From then on, use only the abbreviation. Abbreviations which are common in chemistry (*e.g.* Me for methyl) do not need to be introduced. A list of abbreviations may help the reader when you use many abbreviations.

3.5 Results and Discussion

Of course, the section “results and discussion” is a very important part. Here, you derive and present the outcome of your investigation based on the experimental data. The discussion of the results relates them to a wider chemical context.

This section is often split into separate subsections “results” and “discussion”. This may be appropriate for tightly structured and straightforward experiments. In this case, it is simpler to first report all the results and then add the discussion of these results. However, more complex investigations usually require a series of experiments. Here, the subsequent experiments often depend on the result of the previous ones. Therefore, the reader needs your interpretation of an experiment to understand why you did the subsequent experiment. Therefore, it is advantageous to combine the results and the discussion.

The results and discussion section may vary substantially from organic synthesis to experiments in physical chemistry. Therefore, we can only provide the following general questions and ideas of what you should present as results and discussion:

What are the results?
The primary data usually need to be collected, sorted, transformed, extracted, calculated, plotted, analysed, or interpreted to be of further use. The instructions for the experiment may indicate the necessary data and how to process, extract, and present them. This may include the presentation of a specific absorption band of several compounds in one graph, a least squares fit of collected data points, the identification of an unknown compound, or the comparison of experimental parameters for a series of experiments. Present these data in graphs, tables, figures, or text, as it is most appropriate. It is very important that you do not just analyse the data itself but that you also consider potential experimental errors or even calculate any necessary error propagation.

What did you expect and why?

Presumably, you expressed your expectation already in the introduction as a part of the objectives of the experiment. Here, you have the space to present details, *e.g.* all the data you collected from the literature, chemical considerations, or theoretical calculations.
How do your results compare to your expectations or to theory?
Do both agree or disagree? How significant are agreement or disagreement within the limits of error?

What does it mean? What did you learn?
Relate your results to the objectives of your work. What may be the reasons for success or failure? Do your experiments prove or disprove the initial hypothesis? Do your experiments show that the experimental set-up is working reliably or do you have to improve the set-up? Could you improve an existing synthesis, *e.g.* with respect to yield, or not? Is the applied theory suitable to predict experimental results? In case you find a disagreement, what are potential reasons? Are the expectations wrong and, if yes, why? Are the data in the literature reliable or doubtful? Does the experimental method turn out to be suitable to answer the question under scrutiny? Why is this the case and which other method could be used instead? Are further experiments necessary to test the hypothesis? Can you find a logical explanation for problematic data? What is the most valuable improvement or the most critical part of the experiment?

It is normal that some results appear absolutely clear and other results are more ambiguous or may be interpreted in different ways. Separate both cases clearly (*cf.* sections 4.6.1 and 4.6.2). An ambiguity is no problem as long as you indicate it as such. If there are two conceivable interpretations, present both of them!

Especially in the first laboratory courses, the discussion may be short. Nevertheless, try to pick out some of the questions above and discuss your results. *A good discussion proves that you not just completed the experiment according to the instructions.* Rather, you can demonstrate your interest and your broader chemical understanding through a good discussion! This aspect is important and will be recognised by any reader.

3.6 Conclusion

The conclusion should not be another summary. Often, authors use the conclusion to emphasise their most important findings by repeating them. According to the most cited chemist, *G. Whitesides*, the conclusion "… should add a new, higher level of analysis, and should indicate explicitly the significance of the work."[11] What are the implications of your work beyond your experiment? Do your findings affect other fields in chemistry? Where else can your method be applied? If your results correct data in the literature, what are the consequences? Usually, any solved problem raises new questions. Ask these questions and, if possible, suggest experiments that may answer them.

In most undergraduate laboratory courses, the conclusion may be quite short and nearly indistinguishable from a summary. It is obvious that the idea of an experiment in an undergraduate class is to train students and not to produce new knowledge of general chemical relevance. However, you can present your ideas how to improve your results further or how to improve the most critical parts or weaknesses of your experiment.

3.7 Experimental Section

The main purpose of the experimental section is twofold: First, the description of your experiments should enable any chemist to repeat your experiments and to reproduce your results. Second, any reader should understand what you actually did in the laboratory and how you did it. The reader should find all the data that you acquired, *e.g.* to characterise your products. If not, the reader is not able to follow your argumentation and your interpretation in the results and discussion part of the report. If not, the reader will not accept and acknowledge your conclusions. The best scientific results remain dubious if the reader cannot retrace them because of incompletely or badly described experiments.

The experiments in the laboratory courses span very different areas of chemistry. Obviously, the experimental parts of the reports on the “Simulation of NMR Spectra” and on the “Synthesis of L-3,4-Dihydroxyphenylalanine” will be quite different. For this reason, we focus on general aspects of writing an experimental part. For more information, please refer to the information provided for each specific laboratory course. In addition, the templates for laboratory reports offer further guidance.

It is a good idea to write the experimental part promptly after the execution of the experiments.

First, your memories are fresh, the samples are still available, the computer software may still be running, and so on. Thus, you can supplement important observations that might have evaded your attention. Did you measure the room temperature? Did you make notes of the concentrations of the solutions that were prepared by the teaching assistant? Did you record the type and manufacturer of all of the instruments you used? Did you perform all the necessary characterisation steps of your sample? Remember, you must not use data for your experimental part that is not present in your laboratory notebook! It is very annoying and time consuming if you have to repeat a complex synthesis of a compound only because you failed to complete its characterisation right away. Although the latter aspect may be more important for true research and less in an undergraduate laboratory course, use the laboratory course to train yourself in good practice!

Second, writing down all the procedures, observations, and analytical data for the experimental part helps you to make sure that all pertinent information is available, complete, and understood. This is an indispensable basis for a good report!

Put yourself in the position of a chemist who wants to implement your methods. What you may take for granted may be anything but obvious to others. In case of doubt, rather provide more details than less. Ask yourself: can one implement your protocols by the information that you provide?

Do not abbreviate seemingly boring procedures like this: “… the solution was stirred / heated / extracted / transferred …”. The text has to be short and concise, but still all relevant experimental details have to be given in complete sentences with correct grammar.

It is tempting to copy (more or less) the instructions for the experiment to generate an experimental part. However, you should report what *you actually did* and not what you were supposed to do! Do not use the style of a cooking recipe but write in past tense and passive voice.

Usually, experiments are performed more than once. Reactions have to be repeated because something went wrong in the procedure, new starting material had to be prepared, or reaction parameters had to be varied. Which of the experiments should you report? Describe the most representative (not necessarily the best-yielding) experiment. For a series of experiments (*e.g.* optimisations), summarize the relevant experiments in a table to delineate the parameters that were varied. Only for more complex variations of the experimental details, describe all procedures in full detail.

An experimental part is subdivided in several sections. A general section is provided first. Here, the experimental details that apply for *all* (or at least most) of the experiments are summarized. Depending on the laboratory course and experiment, this general information may be:

- Source and purity of the chemicals and solvents used.
- Generally important information such as working under inert gas atmosphere.
- Instrumentation used, together with details on the employed parameters and the manner of the data presentation.
- Room temperature and ambient pressure.
- Information on computer software.

Do not repeat the information given in the general part in the detailed experimental descriptions. Thus, if "gas chromatography electron impact mass spectrometry" is explained in the general section, then only its abbreviation GC/EI-MS is used in the section of the analytical data, supplemented with the actual data (R_t and MS signals).

A chronological sequence is appropriate for the following sections. Use sub-headings to increase the structure and clarity of your experimental part if necessary. Individual sections may deal with, for example: materials, preparation of starting materials, description of a specific set-up, syntheses, separation, purifying, analytical results, or computational methods.

For syntheses, the title of the section is the complete systematic name of the product according to the IUPAC rules (italics), followed by the formula number of the product (bold; in brackets). Repeat the complete name and the formula number of a compound even if you had already introduced both in the main part. If more than one compound is formed by the reaction, provide the names of all compounds. Nomenclature is sometimes rather difficult and the systematic names may become complex to a degree that the structures behind them are no longer recognized easily. Nevertheless, the systematic names are necessary to avoid ambiguities.

Reactions schemes are very helpful to understand a complex synthesis quickly (see section 4.3). Reaction schemes may be appropriate in the experimental part or in the results and discussion section. Similarly, schematic drawings of a less common instrumental set-up are advantageous.

Enter the quantities of chemicals in brackets after the names of the chemicals. Report the effectively measured quantity (usually mass or volume, net values are sufficient). For substrates and reagents, also report the chemical amount (mol). The latter is not necessary for solvents.

Do not use unspecified temperatures or periods of times such as "room temperature (rt)" or "overnight". Report the measured room temperature and the actual number of hours instead.

Never start a sentence with a numerical value (formula number or measured value).

Use chemical formulae or accepted abbreviations as far as possible, *e.g.* "H_2O" rather than "water", "CH_2Cl_2" rather than "dichloromethane" or "DCM". Some accepted abbreviations are (among others):

- *solvents*: AcOEt, AcOH, Et_2O, MeOH, EtOH, PrOH, *i*-PrOH, *t*-BuOH, DME, DMF, DMSO, THF, MeCN.
- *reagents*: Et_3N, $MeNH_2$, LDA, TMSCl, TBDMSCl, ...
- *groups/substituents*: Ar, Ph, Me, Et, Pr, *i*-Pr, Bu, *t*-Bu, Bn, Ac, Bz, Boc, Fmoc, Z, ….

- *units of physical quantities*: all SI units combined with metric prefixes (*e.g.* km, m, dm, cm, mm, µm, nm, ...), s, min, h, d (for times), ….
- *common instrumentation and related descriptors for data*: m.p., b.p., R_t, R_f, n_D^T, IR (*s, m, w,* br.), UV-Vis (λ_max, λ_min, *sh*), NMR (*s, d, t, q, J*, AB, ….), MS, HPLC, ….
- *abbreviations for procedures* (only for experimental descriptions; not to be used in the body text): soln., aq., sat., conc., dil., …. (consult published papers and sample reports)

Uncommon, specialized, and self-defined abbreviations have to be introduced upon their first appearance in the text. It might be helpful (in particular for larger documents) to include a table with a list of abbreviations. Be restrictive with defining own abbreviations. Do not introduce abbreviations such as rbf (round bottom flask), rf (reflux), or others that you usually do not find as abbreviations in other reports and in publications.

3.8 References

The references section contains a strictly formatted bibliographic list of all sources and literature that you cite in the main body of your report. The bibliography is only one part of the wider subject "citations". Citations are a complex matter. First, not only beginners experience the strict formatting rules, which apply to a bibliography, as time-consuming and annoying. Second, the selection of the literature you cite is related to the sensitive subject "good scientific practice" (*cf.* section 2.2). For these reasons, we refer you to the section 4.5 for more information on references.

3.9 Appendices

Appendices are used for lengthy calculations, large sets of primary data, large tables, extensive spectral data, or anything else that needs to be documented but cannot reasonably be included in the experimental part. Use several and separated appendices for each different type of data you want to append. Use capital roman (upright) letters to number appendices. Include appendices at the very end of your report.

4 Style Guide

4.1 Physical Quantities and Units

The notation of physical quantities and their units is defined by the *International System of Units*.[12] The same notation is specified by the *International Union of Pure and Applied Chemistry* (IUPAC).[13] The most important rules are summarised as follows.

Use italic type for the symbols of physical quantities or variables. For example, write d for diameter, λ for wavelength, or x, y, and z for the *Cartesian* coordinates. This rule can be extended to subscripts and superscripts. Use italic type for the subscript if it denotes another variable (*e.g.* C_V for the heat capacity at constant volume) or a running number (*e.g.* c_i for the concentration of the i-th component). Use roman (upright) type if the subscript is descriptive and not variable (*e.g.* p_CO for the partial pressure of carbon monoxide, T_b for the boiling temperature, V_m for the molar volume).

For vectors, bold and italic type is used. Alternatively, an arrow above the symbol may be used: $\boldsymbol{A} = \vec{A}$.

Use upright type for mathematical functions, constants, or operators: *e.g.* $\ln(x)$, $\sin(\alpha)$, e (the basis of the natural logarithm, *e* in italics would be the elementary charge), i (the square root of minus one, *i* in italics is used for a running number), π (the number Pi), Σ (sum), d*x* for derivatives of *x*.

Units are always given in upright type. This includes any prefixes such as k for kilo or μ for micro. Decimal powers may be used instead of prefixes. Use SI-units and avoid old units such as Torr. Use a capital L for litres to avoid the mix-up of the lower case letter L "l", the number one "1", or a capital i "I", especially in formulae. You may use the small capital ᴍ instead of moles per litre.

Separate several units by blanks to avoid ambiguities: $\mathrm{mmN^{-1}}$ may be metres over milliNewton or millimetres over Newton. Write $\mathrm{mm\ N^{-1}}$ or mm/N or $10^{-3}\ \mathrm{m\ N^{-1}}$ instead. It is good style to use either the notation $\mathrm{mm\ N^{-1}}$ or the notation mm/N consistently. Do not mix both. Avoid expressions with more than one solidus (/), *e.g.* $\mathrm{kg/m/s^2}$. "Per cent" (%) or ppm are also considered to be units although these are multiplication factors in a mathematical sense. In the case your unit is %, make sure that it is clear to the reader what 100 % means.

Numerical values and units are always separated by a blank. The only exceptions to this rule are °, ‘ and “ (degree, minute, second for solid angles). They follow the numerical value without a separating blank. It is a good idea to use the "no-break space" instead of the normal space between numbers and units. This special character prevents the line break between the number and the units. With a normal space, your expression may appear as "10
kg". This does not look professional and it is hard to read. The no-break space is also very useful to prevent a line break within small mathematical expressions. They may appear as $\lambda =$
635 nm otherwise.

Use the "true" minus sign "−" (Unicode 2212) for the mathematical operator minus instead of the hyphen "-". The true minus sign corresponds to the plus sign in width and vertical position (compare "− +" and "- +"). The hyphen is very short and often hardly visible as a minus sign, especially in superscripts. The true minus sign is equal to the minus sign that is used by formula editors. Finally, the true minus sign prevents a line break within your expression. $\lambda = 6.35\cdot10^{-}$
^{7} m may be the unpleasant result of using a hyphen as minus sign.

Use the special characters · or × as operators for multiplication. Do not use the star * or the letter x (*cf.* section 5.4 on how to access these special characters easily).

A physical quantity is the product of a numerical value and a unit. This can be used for quantity calculations. Consider the distance $d = 52\ \mu\mathrm{m}$. Obviously, the expression $d/\mu\mathrm{m} = 52$ is also correct mathematically. One could also write $d = 5.2\cdot10^{-5}\ \mathrm{m}$ or $d\cdot10^{5}\ \mathrm{m^{-1}} = 5.2$. These transformations are very useful in order to find the correct head of a column in a table (*cf.* section 4.2). In columns one and two of Table 1, the distance *d* is given in the units of μm and m according to the above examples.

$d/\mu\mathrm{m}$	$d\cdot10^{5}\ \mathrm{m^{-1}}$	$10^{-3}\ T/\mathrm{K}$	$10^{6}\ K/\mathrm{T}$
52	5.2	3	30

Table 1. Example of scientifically correct table heads.

Columns 3 and 4 further exemplify how to read values in a table. For column 3 we can write $3 = 10^{-3}\ T/\mathrm{K}$. Solving the equation for the temperature *T* results in $T = 3000$ K. The comparison of columns 3 and 4 demonstrates how important the correct type is. In column 4, a quantity K is given in units of Tesla: $K = 30\ \mu T$.

We are aware that several different notations for table heads are in use, *e.g.* "d in µm", "d [µm]", or "d (µm)". Although these are comprehensible, we require you to use only the notation recommended by the IUPAC.[13] The same rules as for table heads have to be applied when finding the correct labels of axes in plots (*cf.* section 4.3.3)!

Every physical quantity is subject to some uncertainty that is mostly of experimental origin. Consider and determine this uncertainty wherever necessary and specify it. Use the notations

$$l = 4.328\ \text{m} \pm 0.004\ \text{m or}$$
$$l = (4.328 \pm 0.004)\ \text{m}.$$

Make sure that you specify how you determined the uncertainty. Do you use the standard uncertainty σ or 3σ or any other value?

Report numerical values with a meaningful number of significant digits. It is senseless to report a length up to the digit representing mm, as in $l = 4.318$ m, when the experiment does not allow a precision better than 1 dm. Round accordingly and report $l = 4.3\ \text{m} \pm 0.1\ \text{m}$.

4.2 Tables

Tables are used to present many numerical values that are systematically related. Understanding the content of a table takes time. Therefore, use a table only when the numerical values themselves are important (*e.g.* for look-up purposes). If you just want to show that one quantity increases as a function of another quantity and exact values are not important, use a graphical presentation instead.

Do not use tables for small amounts of data. For example, the data in any 2 by 2 table is preferably presented as plain text. For large amounts of data, the table may span more than one page. In this case, repeat the column heads of the table on every page. Avoid page breaks within a table wherever possible. Consider to place large tables in the appendix.

Refer to all tables by callouts in the text. For example: "Table **Fehler! Verweisquelle konnte nicht gefunden werden.** summarizes the measured data". Place the table close to the position of the first callout.

Number all tables consecutively and place the table caption above the table.

Table **Fehler! Verweisquelle konnte nicht gefunden werden.** provides an example for a mediocre table. Clearly, the presentation of the data and the formatting of the table can be improved. (Only layout and presentation of the data are of interest. The numbers itself do not have any physical or experimental meaning.) In Table **Fehler! Verweisquelle konnte nicht gefunden werden.**, all the issues discussed in the following are improved.

The grey background of column one and row one is not necessary. On a computer screen, the text may appear legible. However, after printing and copying, the contrast may be too low. Use black type on white background.

Using all possible grid lines is not wrong but also not necessary and unpleasant for the eye. Just compare the optical appearances of Tables **Fehler! Verweisquelle konnte nicht gefunden werden.** and **Fehler! Verweisquelle konnte nicht gefunden werden.**. Using a head rule, a neck rule, and a foot rule is sufficient. This format is also used by many scientific journals.

Table **Fehler! Verweisquelle konnte nicht gefunden werden.** uses *Times New Roman* as font. This is not wrong. However, a font without serifs may appear plainer and more functional in a table (*cf.* section 4.3).

The notation of the quantities and their units in the first row differs from column to column. Nearly all table notations in row one ignore the rules presented in chapter 4. The notation Γ (mmol / m^2, $\cdot$ 10^{-3}) is confusing. Why use the prefix m for milli *and* a factor of 10^{-3}? In addition, the non-mathematical separation by a comma makes the reader unsure. Are the values to be multiplied by 10^{-3} or did the author do that already? Such uncertainty and ambiguity must be avoided!

Table 2. Data for my experiments.

solu-tion	***c* [mM]**	**ln (*c*)**	***V* in l**	**Δ*V* in mL**	***γ* / mN / m**	***Γ* (mmol / m^2,·10^{-3})**
0	200	−1.609	0.005	1	< 35	0.6
1	40	−3.219	0.005	1	34.8	−0.8
2	8	−4.828	0.010	1	35.6	0.9
3	1.6	−6.438	0.010	1	38.2	2.1
4	0.32	−8.047	0.050	1	45.7	6.4
5	0.064	−9.657	0.050	1	68.2	3.1
6	0.0128	−11.266	0.050	1	71.9	0.2
7	0.00256	−12.876	0.100	1	72	0.06
8	0.000512	−14.485	0.100	1	72.1	0.04

The first value for γ in column 6 is "< 35". First, only one half of an inequality may be misleading because the missing half of the inequality is unclear. Second, the true value in this example can range between minus infinity and 35. Is this information useful? There may be reasons for not having one clear value. In such a case, it is better not to report any inequality but to state the reasons why no value is reported.

Column 5 for Δ*V* is useless because all the values in all rows are identical. The error of the volume could be given as a footnote in the table, in combination with any error calculations (if present), or in the experimental part.

The values for the volume in column 4 are ok but not very convenient to read. The numbers can be understood faster when you present them in the common unit of mL. It is inconsistent to use a lower case "l" and a capital "L" for litres in columns 4 and 5.

The values for the concentration *c* in column 2 span several orders of magnitude. In this case, it is impossible to present values that are convenient to read. Here, it is a good idea to use the most common unit in the head of the column and use decimal powers in the table.

Using the unit M = mol L^{-1} for *c* also solves the problems in column 3. According to the head the logarithm of *c* is given. However, the logarithm of 200 cannot be negative. Closer inspection reveals that units of mol L^{-1} are used for the calculation of the logarithm although mmol L^{-1} are used in column 2. This is an unnecessary and confusing inconsistency. A second problem is the occurrence of a unit in the logarithmic expression ln(*c*). The logarithm of any unit is not defined. Using thermodynamically exact formulae (units never appear in a logarithm in thermodynamically exact formulae) solves both problems. The correct expression for column 3 may be $\ln(c/c^\ominus)$ with the standard concentration $c^\ominus = 1$ mol L^{-1}.

Finally, the caption of Table **Fehler! Verweisquelle konnte nicht gefunden werden.** is not very useful. A good caption provides a short but helpful description of the content of the table and contains necessary information to read the table. It should not repeat the main text. Avoid page breaks within a table. If your table is too large to be printed on one page, repeat the header on every page. Check the final and printed version for the layout of tables.

Table 3. Summary of the prepared solutions, their concentrations *c*, the logarithm of the concentration *c*, the used volumes *V* of the solutions, the measured surface tension γ, and the calculated surface excess Γ. [a] The error of the volumes was ±1 mL for all solutions. [b] Formation of foam prevented a reliable measurement.

soln.	c/M	$\ln(c/c^\ominus)$	V/mL[a]	$\gamma \cdot 10^3$ m N^{-1}	$\Gamma \cdot 10^6$ m^2 mol^{-1}
0	$2 \cdot 10^{-1}$	−1.609	5	–[b]	0.6
1	$4 \cdot 10^{-2}$	−3.219	5	34.8	−0.8
2	$8 \cdot 10^{-3}$	−4.828	10	35.6	0.9
3	$1.6 \cdot 10^{-3}$	−6.438	10	38.2	2.1
4	$3.2 \cdot 10^{-4}$	−8.047	50	45.7	6.4
5	$6.4 \cdot 10^{-5}$	−9.657	50	68.2	3.1
6	$1.28 \cdot 10^{-5}$	−11.266	50	71.9	0.2
7	$2.56 \cdot 10^{-6}$	−12.876	100	72.0	0.06
8	$5.12 \cdot 10^{-6}$	−14.485	100	72.1	0.04

4.3 Schemes and Figures

“A picture is worth a thousand words” summarises nicely that any kind of artwork is a very powerful tool to convey information. Artwork can be any kind of drawing, scheme, graph, sketch, image, presentation of 2D- or 3D-data, line art, photograph, or combinations thereof. Creating artwork is a complex endeavour. First, there are many different sources of data for artwork. Second, there are even more programs and means to create or modify artwork. Finally, many different digital formats exist. Therefore, we forgo general instructions on artwork which you can find in the literature.[14,15] Instead, we concentrate on the two most important types of artwork for laboratory reports: schemes and figures.

4.3.1 General Considerations

An illustration is superior to plain text when it helps the reader to understand a certain part of your work much faster or more easily. A good illustration is clear, focusses on the important things, is legible, and does not confuse the reader because of a bad design, less relevant details, or a bad description of the illustration in the text.

It is a good idea to sketch your illustration by hand first to select the best design of the overall figure. Before you start to design the scheme or figure on a computer, consider the final size of your graphics in the finally printed document. Small lettering or very thin lines may reproduce too poorly to be legible. Plan the size of symbols and fonts and the line widths accordingly and test it by printing your graphics in their final size. This is especially important when the size of the whole page may be reduced (*e.g.* from DIN A4 to DIN A5).

Your illustration should be legible after printing or copying. This requires good contrast. Therefore, use dark colours on white background and avoid grey lines, grey text, grey axes, or grey background. You may use colour as a valuable means to add information. However, colour may turn to grey by printing or copying. In addition, colour-blind people should be able to read your graphics. For lines, you can avoid this problem by the use of different line styles (dotted, dashed …) in addition to colour.

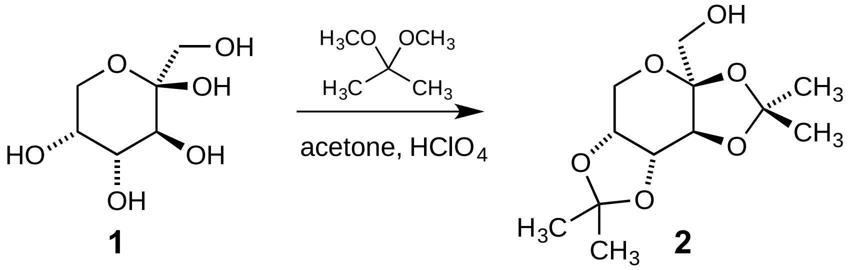
Use only one font (plus symbols if necessary). Choose a font without serifs, preferably a common font like *Helvetica* or *Arial*. Do not use more than two different font sizes. Fonts with serifs, too many different fonts, or several font sizes make your figure look cluttered.

Refer to all graphics by callouts in the text. Place the graphic close to the position of the first callout. Number all graphics consecutively with Arabic numerals as they appear in the text. Number figures and schemes separately and independently from each other.

Whatever type of graphics you include in the report, you still have to guide the reader through your graphics step by step in full sentences! It is insufficient to write "The relevant data is shown in Fig. 1" without further explanation and let the reader extract whatever he may find in Fig. 1. Instead, introduce a new figure with one sentence like "The extinction coefficients of compounds **1** to **5** are plotted in Fig. 1 as function of the wavelength." Then, explain the simplest issue in your figure. For example, start with the standard sample or any reference signal. It is quite easy to develop your description of the figure from this starting point.

4.3.2 Schemes

There is no clear differentiation between figures and schemes. Some journals use the designation "figure" for all types of graphics exclusively. For your laboratory reports, label two types of illustrations as schemes: reaction schemes to present a single or several consecutive chemical reactions and flow chart diagrams. Thus, schemes contain "arrows". Scheme 1 provides an example for a reaction scheme. We demand you to use the program *ChemDraw* and the style sheet that you used in the GPC (http://www.chem.uzh.ch/bienz/lecture/gpc/Files/). The parameter settings in this style sheet ensure a good presentation. Note that some journals offer files with settings for the program *ChemDraw* on their homepage to match the specific requirements of the journal.



Scheme 1. Synthesis of 2,3:4,5-Di-*O*-isopropylidene-β-D-fructopyranose (**2**).

4.3.3 Figures

Any illustration that is not a scheme is termed figure. Apart from the general considerations in section 4.3.1 we refer you to the literature for further general guidelines.[14,15] Here, we restrict ourselves to the most frequent types of figures: structural formulae and graphs.

It is customary to introduce chemical compounds, their structural formulae and corresponding formula numbers in a figure as in Fig. 1. Use the style sheet as introduced in the GPC.

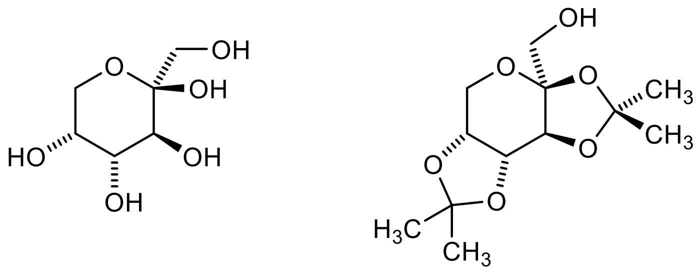
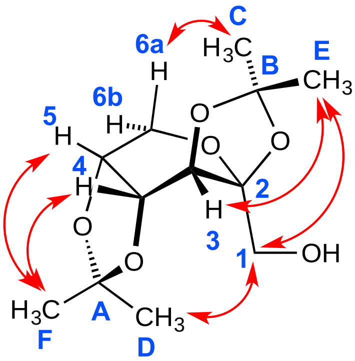


Figure 1. Structural formulae of β-D-fructopyranose (**1**) and 2,3:4,5-di-*O*-isopropylidene-β-D-fructopyranose (**2**).

Fig. 2 provides a more elaborate example of a figure including a structural formula.



2

Figure 2. NOESY correlations that are relevant for the structural proof of compound **2** and the assignments of the individual ^{1}H-NMR signals.

Apart from structural formulae, graphs will be prevalent in your reports. As an example, let us assume you measure an absorption spectrum. Two peaks overlap. You fit the sum of two individual peaks to the experimental data. Finally, you want to display everything graphically.

Mathematical plots or similar figures should be as clear and as self-explaining as possible. These requirements are not quite fulfilled by Fig. 3, which gives an example how the output of a standard spreadsheet software may look like. You may use *Excel* or similar programs. However, keep in mind that these programs are primarily designed for accounting and less for scientific purposes.

To maximize clarity, avoid any unnecessary components. Use minor tick marks, grid lines, or frames only if they are necessary to read the plot. Avoid explanatory labels ("outlier" in Fig. 3), insets, or legends in the plot itself unless they are truly necessary to understand a specific feature. In this example, the experimental part may provide the information, how you treated outliers during the data analysis. The legend in Fig. 3 reduces the space which is available for the plot itself (note that Fig. 3 is of the same overall size as Fig. 4). Instead, provide necessary information in the caption. Scale the axes such that you use the available space efficiently.

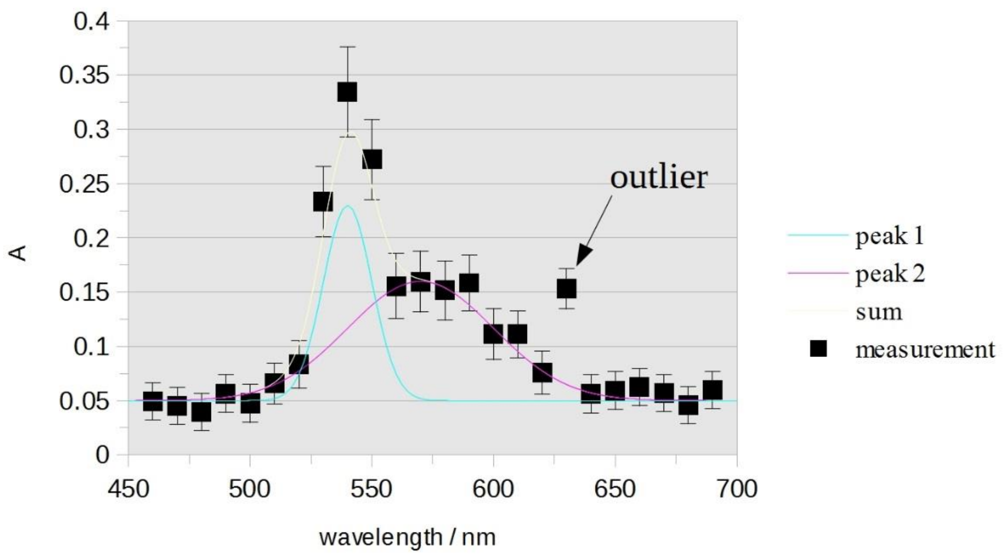


Figure 3. Standard output of common spreadsheet software.

Fig. 4 provides an improved representation. In addition to the guidelines in section 4.3.1, consider the following points.

Choose visual cues of appropriate size, shape, and colour for different sets of data such that they are easy to distinguish. Explain them by identical visual cues in the caption.

Make sure that the labels of the axes are labelled in accordance with the rules in section 4.1. The combination of prose and mathematic notation in “wavelength / nm” in Fig. 3 is questionable.

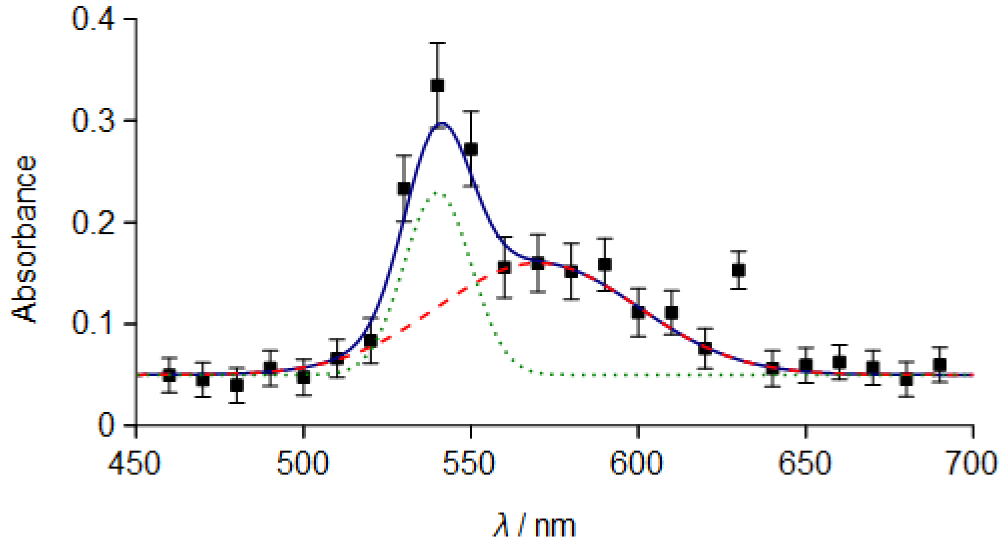


Figure 4. Absorbance spectrum of compound **9**. The error bars of the measured data (■) correspond to the standard deviation after averaging. The spectrum was fitted (continuous blue line) as sum of two *Gaussian* peaks centred at 540 nm (dotted green line) and 570 nm (dashed red line).

If your plot contains error bars, make sure you provide their meaning (*e.g.* range of observed values, 1σ, 2σ …) in the caption or wherever appropriate.

If you use a pre-formatted output for graphs from other sources, *e.g.* spectrometer software, the style may not conform the rules above. In this case, it is not necessary to re-format the graph for your laboratory report. However, re-formatting may be necessary for a publication or thesis!

4.4 Analytical Data

Analyses of chemical compounds are prevalent in chemistry for obvious reasons. Therefore, the proper presentation of analytical data is very important. Contrary to the rules defined in section 4.1, it is customary to omit the unit of a physical quantity to save space (repeating the unit of cm^{-1} after 23 signals of a spectrum is not necessary). However, make sure that you report your data according to common standards or provide a clear note on the units you use in the general section of the experimental part. For historical reasons, also non-SI units are customary.

The purpose of the analytical methods may vary in our laboratory courses. Therefore, the amount of data that you have to report may vary (*e.g.* all signals of an IR spectrum, merely the diagnostic or characteristic signals, or only one signal as function of time). Check the instructions of the experiment or the laboratory course for more information.

Report your analytical data in the sequence of the following sections. Create subsections for each analytical method if your analytical part is long. Follow the examples provided in the subsequent sections. If the acquisition of any of the data is inappropriate or not possible, provide a scientifically well-founded statement as explanation. For instance, an optical rotation value, $[\alpha]_{\mathrm{D}}^{T}$, value makes only sense for an optically active (enantiomerically enriched) compound. UV-Vis spectroscopy is only appropriate for a compound with a chromophore. In such cases, you may write:

> $[\alpha]_{\mathrm{D}}^{T}$,: achiral (or racemic).
>
> UV-Vis: no chromophore.

4.4.1 Appearance

Characterize the samples by their aggregation state and colour. Distinguish white (*e.g.* a powder, a precipitate, *etc.*) and colourless (*e.g.* crystals, liquids, *etc.*). Add further attributes if appropriate. Provide the viscosity for liquids. For solids, describe the appearance as detailed as possible (amorphous *vs.* crystalline, add the habit of the crystals).

> “colourless highly viscous liquid.”; “slightly yellowish oil.”; “brownish, like varnish.”; “off-white needles.”; “colourless, rhombic.”

4.4.2 Purity

The quality of a sample is characterised either by its purity or by content. Purity is a relative measure determined by a specific method (*e.g.* the percentage of the area of the product peak in HPLC). Purity does not quantify the absolute amount of the product in a sample. An absolute quantity is the mass fraction or content (in percent), which is not trivial to determine. Report the purity to characterise the quality of your sample unless the contaminations are known.

> “Pure according to TLC.”; “Purity: 96 % (HPLC, 210 nm)”; “Purity: 98 % (GC/EI-MS).”; “Purity: >95 % (^{1}H-NMR).”
>
> “Content: 95 %, contaminated with 5 % of starting material.”

4.4.3 Chromatography

Provide the chromatographic conditions in addition to the R_f values (TLC) or the R_t values (GC, HPLC). Usually, the type of TLC plates and the instrumentation used for HPLC is described in the general section of the experimental part. Thus, add only the missing information, *e.g.* the solvent system for the TLC, the solvent system (gradient if applicable), the type of column, the flow rate, or the detection method for the HPLC.

> TLC: R_f = 0.67 (AcOEt/hexane 5:1).
> GC: R_t = 3.23 min.
> HPLC: R_t = 4.73 min (5 mm × 20 cm RP-18 column, MeCN/H_2O 1:10, flow rate 1.0 mL min^{-1}, detection at λ = 210 nm).
> HPLC: R_t = 7.88 min (5 mm × 20 cm *Chiracel-OD1*, MeCN/H_2O 1:10 for 5 min, gradient to MeCN/H_2O 5:10 for 10 min, flow rate 1.0 mL min^{-1}).

4.4.4 Refractive Index, Boiling Point, and Melting Point

Report the refractive index n_D^T with four digits after the decimal point. Compare your value with data from the literature, if available.

> n_D^{23} = 1.3638 (lit.: 1.3641[27]).

You do not have to measure the boiling point (rather boiling range) of a compound with a special apparatus. If you distilled a compound, the b.p. is the range of the head temperatures that you observed when the compound distilled over. If you cannot measure the head temperature (*e.g.* in *Kugelrohr* distillations), report the air bath temperature and indicate the temperature correspondingly. Supplement the observed boiling range with the pressure at which the distillation was performed. If available, compare your values with data from the literature. Use the same units and comparable conditions for your measurements.

> b.p.: 122–124 °C ($4\cdot10^{-2}$ mbar, lit.: 130 °C ($4\cdot10^{-2}$ mbar)[12]).
> b.p.: 125–130 °C (air bath temp., 4 Pa, lit.: 130 °C (5 Pa)[27]).

Use a heating rate of 2 °C min^{-1} for the determination of the melting point (rather melting range). The lower limit of the range is reached when two thirds of the material is molten (to be estimated) and the upper limit when all the material is liquid. Supplement the observed melting range with the solvent from which you recrystallized the sample (alternatively, from where the solid was collected) and compare your data with literature values if available.

> m.p.: 135–136 °C (H_2O/MeOH, lit.: 134 °C (H_2O)[12]).
> m.p.: 128–131 °C (after chrom. upon evaporation of the solv., lit.: 134 °C[27])

4.4.5 Specific Rotation

Report the specific optical rotation $[\alpha]_D^T$, the solvent, and the concentration of the sample solution (in g per 100 mL for historical reasons). It is imperative that you denote the algebraic sign (+/−) of the rotation explicitly. Supplement values from the literature if available.

> $[\alpha]_D^{23}$ = +15.8 (c = 0.1, MeOH), lit.: −16.0 (c = 0.2, MeOH, enantiomer).[27]

4.4.6 UV-Vis Spectra

Provide the solvent that you used for the measurement in brackets next to the method. List the wavelengths λ at which maxima (max), minima (min), or shoulders (sh) appear in ascending order in units of nm. For the sake of brevity, the unit nm may be omitted after the numerical value. The values for the wavelengths are followed by the respective values of log(ε).

UV-Vis (MeOH): λ_{max} 200 (4.50), λ_{min} 239 (0.56), λ_{max} 259 (2.20), λ_{sh} 269 (1.60).

4.4.7 IR Spectra

List the signals of an IR spectrum by descending wavenumbers (1/λ) in units of cm^{-1}. Round wavenumbers to the next integer. Each wavenumber is followed by a letter that indicates the relative intensity at this wavenumber (*s*, *m*, and *w* for *strong*, *medium*, and *weak*). For diagnostic signals, add the respective structural units (*e.g.* O–H, C=O, C=C, or arom., C–H of aldehyde, *etc.*) in brackets. Indicate the shape of particularly broad signals by "(br.)" (*e.g.* O–H bands of hydrogen-bridged alcohols or acids). Add the type of the sample (neat film between NaCl plates, ATR, KBr pressling, or solution) only if you did not define it in the general section of the experimental part. IR ($CHCl_3$): 3614*m* (free O–H), 3387*s* (br., O–H, H-bridge), 3083*w*, 3062*w*, 3030*w*, 3001*w*, 2956*m*, 2923*m*, 2871*w*, 1782*s* (C=O), 1708*s* (C=O), 1604*m* (C=C, arom.), 1583*m* (C=C, arom.), 1495*m*, 1481*w*, 1453*m*, 1443*w*, 1387*s*, 1348*s*, 1291*m*, 1262*s*, 1212*s*, 1203*s*, 1172*m*, 1101*m*, 1076*m*, 1047*m*, 1031*m*, 1012*m*, 1002*w*, 978*m*, 919*w*, 873*m*.

4.4.8 ^{1}H-NMR Spectra

Report the signals of a ^{1}H-NMR spectrum in the following order: chemical shift (report the δ range for multiplets), multiplicity (italicised and in brackets), the coupling constant(s) in Hz, the number of hydrogen atoms, and the interpretation. Order the signals in descending order of chemical shift and separate signals by a semicolon. Separate signals with a mutual interpretation by a comma instead (*cf.* the *AB* system in the example).

Describe well-structured multiplets as detailed as possible to give the reader the best idea of their appearance. For instance: "3.50 (*d*-like *m*, "*J*"= 7.0, CHOR)" or "4.74–4.52 (symm. *m*, 8 distinctive lines, *X* portion of an *ABX* system, CHOR)".

Report chemical shifts to two decimal places and coupling constants to one decimal place. If you observe more than one coupling (*e.g.* in a *dt* or a *td*), list the values for *J* in descending order. Order the multiplicities according to the order of the coupling constants to avoid mis-interpretation! Thus, (*dt*, *J* = 7.3, 3.4, ...) means that you observed a proton signal with a *d*-splitting of 7.3 Hz and a *t*-splitting of 3.4 Hz, while (*td*, *J* = 7.3, 3.4, ...) means that the *t*-splitting is 7.3 Hz and the *d*-splitting is 3.4 Hz.

Use structural units (rather than carbon numbers derived from nomenclature) for the assignment of the signals. For larger molecules or molecules with repetitive structural motifs, it is advisable to introduce a generic structure with generic numbering of the atoms. If the exact number of responsive H-nuclei is obvious from the structural unit, do not provide the number of hydrogen atoms separately. Use italics to assign the H-atoms in larger structural units unequivocally.

> ^{1}H-NMR: 7.39–7.20 (*m*, 5 arom. H); 5.94 (*dd*, J = 9.6, 6.3, BrHC); 4.71–4.62 (*m*, HCN); 4.28–4.16 (*m*, H_2CO); 3.41 (*dd*, J = 13.3, 3.4, 1 H, PhCH_2); 2.85, 2.83 (*AB*, J = 13.4, $ClCH_2$); 2.71 (*dd*, J = 13.3, 10.3, 1 H, PhCH_2); 1.98 (*dd*, J = 14.5, 9.6, 1 H, $SiCH_2$); 1.66 (*dd*, J = 14.5, 6.3, 1 H, …

4.4.9 ^{13}C-NMR Spectra

Report the signals of the ^{13}C-NMR spectrum analogously to the signals of the ^{1}H-NMR spectrum in descending order of their chemical shifts. Provide the multiplicities derived from DEPT-135, DEPT-90, or HSQC experiments in brackets and italicised (without coupling constants), followed by the interpretations. Including the number of carbon atoms unless this number is equal to one. Separate the descriptions of individual signals with a semicolon. Use a comma for the separation of signals with a mutual interpretation (*cf.* the signals at 129.4 ppm and 129.1 ppm in the example). Report the chemical shifts to one decimal place, except when two signals were identical. In such a case, report two digits after the decimal point.

> ^{13}C-NMR: 169.6 (*s*, CON); 152.5 (*s*, COO); 135.0 (*s*, arom. C); 129.4, 129.1 (2*d*, 2 × 2 arom. C); 127.5 (*d*, arom. C); 66.4 (*t*, H_2CO); 56.1 (*d*, HCN) 41.5 (*d*, BrHC); 37.9 (*t*, PhCH_2); 30.0 (*t*, $ClCH_2$); 21.3 (*t*, $SiCH_2$); …

4.4.10 MS Spectra

In contrast to the spectroscopic methods above, you do not need to report all peaks of an MS spectrum. The signal of a molecular species in MS usually consists of a peak group that derives from the several isotopologues the structural unit is composed of. Report only the monoisotopic peaks and omit the isotopologues for routine MS spectra. However, report the isotopic pattern if it is of diagnostic relevance, as it is the case for Cl- or Br-derivatives (*cf.* second example). For low-resolution MS, report the *m/z* value with the nominal mass (usually the measured *m/z* value rounded to the next integer). The relative intensities in percent follow in brackets. Provide an interpretation of the signals as far as possible. Arrange the signals in descending order of their *m/z* values, separated by a comma. For GC/EI-MS, report the retention time of the chromatographic peak that is analysed by MS (*cf.* example).

The interpretation of the base peak and of the signal of the highest observed mass (usually the signal of the molecular ion, the ionised molecule, or an adduct ion) is mandatory. In addition, interpret all of the ion signals that are due to common fragmentation reactions such as the α–fission, *McLafferty* rearrangement, onium reaction, or CO loss.

By convention, use the notation $M^{+\bullet}$ for molecular ions. Ionised molecules (adduct ions, obtained with other ionisation methods than EI) and fragment ions are written as $[M + H]^+$, $[M + Na]^+$, $[M - H]^-$, and $[M - C_xH_y]^+$ or $[M - C_xH_y]^{+\bullet}$ (depending on the fragment that is lost). Do not overly interpret the spectra. Give structures and formulae only for those fragments that you can safely explain.

> GC/EI-MS (R_t = 3.6 min): 72 (25, $M^{+\bullet}$), 57 (8, $[M - CH_3]^+$), 43 (100, $[M - C_2H_5]^+$), 29 (17, $[C_2H_5]^+$), 27 (8).
> CI-MS (NH_3): 439/437/435 (30/100/73, $[M + NH_4]^+$), 357 (9), 338 (6, $[M - Br]^+$), 249 (30), 195 (9) 164 (28), 147 (34), 115 (9).

For high-resolution, high-accuracy MS, report the ion mass exactly as measured, the proposed ion composition, the respective theoretical mass and the mass deviation (in ppm).

> HR-ESI-MS (MeOH): 184.09689 (100, $C_9H_{14}NO_3^+$; $[M + H]^+$; calc. 184.09682; Δ = 0.39 ppm).

Consult the literature for the description of other MS spectra, *e.g.* for MALDI-MS, HR-MS, or MS/MS.[16]

4.4.11 Magnetic Susceptibility

Report the calculated value μ_{eff} in units of μ_B together with the state of the measured sample solid, liquid, or solution) and the temperature of the measurement. In addition, indicate the number of unpaired electrons and the spin state of the sample metal.

> Magnetic Susceptibility (neat solid, 23 °C): μ_{eff} = 5.91 μ_B (5 unpaired electrons; high-spin).

4.4.12 Elemental Analysis

There are several methods available for the determination of elemental compositions of compounds. We concentrate here on the combustion analysis for CHNS, and on potentiometry and complexometry, respectively, for the quantification of specific cations and anions.

For combustion analyses, report the chemical formula of the proposed analyte, its molecular mass as well as the theoretical mass percentages of the measured elements to two decimal places. Use all reliably available digits of the atomic masses for the calculation. Then, list the experimentally found values. The maximum allowed deviation is 0.4 % (absolute).

> Anal. calc. for $C_{16}H_{21}BrClNO_3Si$ (418.79): C 45.89, H 5.05, N 3.34. Found: C 45.72, H 5.13, N 3.29.

For potentiometry, report the ion to be quantified, the composition of the medium of measurement, the chemical formula of the proposed analyte, its molecular mass as well as the theoretical mass percentage of the measured species to two decimal places. Use all reliably available digits of the atomic masses for the calculation. Then, list the experimentally found value.

> Potentiometry of Cl^- (KNO_3, 0.1 M in H_2O) calc. for $Cl_3CoH_{18}N_6$ (267.47): Cl 39.76. Found: Cl 39.59.

For complexometry, report the ion to be quantified, the indicator and the composition of the titrant solution, the chemical formula of the proposed analyte, its molecular mass as well as the theoretical mass percentage of the measured ion to two decimal places. Use all reliably available digits of the atomic masses for the calculation. Then, list the experimentally found value.

> Complexometry of Co^{3+} (murexide; EDTA, 0.1 M in H_2O) calc. for $Cl_3CoH_{18}N_6$ (267.47): Co 22.03. Found: Cl 21.99.

4.5 References and Citations

4.5.1 Types of Quotations

There are three types of quotations: direct quotation, indirect quotation, and block quotation.

The indirect quotation is most often used in scientific texts. Most of the citations in this handbook are indirect quotations. You refer to the meaning or content of the quoted work, but you do not copy any phrases literally. Use your own words if you want to summarise the content of the quoted work.

The direct quotation is used to repeat an exact phrase or sentence of an author. The maximum length of a direct quote is a few lines. An example is the well-known final sentence of the publication by *Watson* and *Crick* on the structure of DNA:“ It has not escaped our notice that the specific pairing we have postulated immediately suggests a possible copying mechanism for the genetic material.”[17] The quoted text must be marked by quotation marks or inverted commas. You must not change the quoted text in a direct quotation even if you have to copy misprints! You may indicate the exact copy by adding (*sic*) after the quotation. *Sic* is the abbreviation of the Latin phrase *sic erat scriptum*, which means “thus it was written”.

A block quotation is similar to a direct quotation, but it is used for long texts or entire paragraphs which exceed a few lines. The quoted text has to be distinguishable from the normal text by using blank lines to separate it and by using a different font, size, or typeface.

Be aware that the work of others may be protected by copyright! This is especially true for block quotations and all kind of graphics or images. You may reproduce a protected image but this requires special permission from the author or the publisher of the original work.

4.5.2 Technical Aspects of Citing

Unfortunately, there exist hundreds of styles how to cite literature even within a single scientific field.[5] They differ from publisher to publisher and from journal to journal. A consequence is that the citations have to be re-formatted once a manuscript is rejected by one journal and has to be submitted to another journal. A standard publication contains approximately 40 citations, whereas this number may exceed 200 in a review article! Naturally, most authors consider the work of re-formatting citations an unnecessary and annoying obstacle. Fortunately, modern citation management software can perform most of this work.

In your first laboratory reports, you may need only very few citations. Sorting, referencing, and formatting a few citations “by hand” is of course feasible. Presumably, formatting manually is even faster than learning how to use citation management software. However, we strongly recommend that you use citation management software from the beginning for two reasons:

First, use the first laboratory reports to get used to citation management software. You will need this software latest when writing your bachelor thesis. Here, the number of citations will be high, and several rounds of editing will shuffle your citations repeatedly. Therefore, formatting by hand is no longer a reasonable option. If you start to learn how to use citation management software only during writing your bachelor thesis, you are in severe danger of running out of time.

Second, modern and professional citation management software allows much more than sorting, numbering, and formatting of citations. For each citation, you can automatically collect PDF-files, add your ideas and questions, add your personal key words, rate publications according to your own measures, link it to files or web resources, or manage open tasks to name only a few possibilities. Managing literature like this results in a very valuable, personal, and digitally searchable database of literature. Because this is a long-term investment, it is a very good idea to start as early as possible! Without such knowledge management, it is very hard to have or maintain an overview of the literature.

As you should concentrate on the more scientific issues of writing a laboratory report instead of losing time because of formatting and re-formatting your bibliography, we require you to use the citation style of the journal *Angewandte Chemie International Edition* in all initial laboratory courses. In addition to the basic explanations below, you can find the guidelines in the literature.[18] (In later courses, you may be required to follow the guidelines of a different journal for training purposes.)

A complete citation consists of two parts. The first part is a reference in the text. The second part is a corresponding entry in the bibliography in the references section of your report (*cf.* section 3.8).

The reference in the text indicates that you are citing and the number in this reference refers to the corresponding entry in the bibliography. Use a superscript Arabic number in square brackets for the reference in the text. Number your references according to their appearance in the text. The square brackets prevent confusion with other superscripts such as mathematical exponents. Place the reference directly after any punctuation unless a citation in the middle of a sentence is necessary. One reference in the text may refer to more than one entry in the bibliography. In this case, separate the numbers by a comma without blank. Combine a range of consecutive numbers by a dash if first and last number differ by more than two. Examples: “A similar method was reported for silicon,[1] aluminium,[1,2] zirconium[2–6,10], and titanium.[8,9,12]”

A specific feature of the style used by *Angewandte Chemie International Edition* are composite references. Instead of, for example, three single entries in the bibliography ”[5–7]“, these three references are combined to one reference in the text ”[5]“. Entry 5 in the bibliography lists all three citations denoted by a), b), and c). Any reference to single entries of a composite reference is given in the text as [5b] or [5a,6a,23a–e]. You may forgo to use composite references. You do not need to worry about this if you use citation management software with a properly implemented citation style of *Angewandte Chemie International Edition*.

All entries in the bibliography must refer unambiguously to the original work. In addition, the list of citations in a publication must be readable to computer programs for purposes of citation analysis, citation counting, and automatic linking. For both reasons, the list has to be formatted according to strict rules including punctuation and typeface. We recommend again using a citation management software for formatting the bibliography.

It is unnecessary to describe the formats of all types of citations in detail. These can be found in the literature.[18] Much more instructive and as useful are examples for the most frequent types of literature you will have to cite:

Journal article:

> [1] A. L. Sumner, E. J. Menke, Y. Dubowski, J. T. Newberg, R. M. Penner, J. C. Hemminger, L. M. Wingen, T. Brauers, B. J. Finlayson-Pitts, *Phys. Chem. Chem. Phys.* **2004**, *6*, 604–613.

Note that the titles of all journals are abbreviated. Unfortunately, different fields in science use different rules for the abbreviation. The abbreviations common in chemistry can be retrieved from the Chemical Abstracts Service Source Index (CASSI).[19]

A unique document identifier (DOI) is assigned to every journal article. This DOI can be used to cite a journal article that has not yet been published in printed form (volume and page number are not yet available) but is already accessible online.

[1] D. T. Simon, E. O. Gabrielsson, K. Tybrandt, M. Berggren, *Chem. Rev.*, DOI 10.1021/acs.chemrev.6b00146.

Books without editor:

[1] M. Hillert, *Phase Equilibria, Phase Diagrams and Phase Transformations: Their Thermodynamic Basis*, 2. ed., Cambridge University Press, Cambridge, **2008**, p. 13.

Books with editor:

[1] S. Austin, A. Glowacki in *Ullmann's Encyclopedia of Industrial Chemistry, Vol. 18* (Ed.: B. Elvers), Wiley–VCH, Weinheim, **2011**, pp. 191–205.

In case there are more than one editors, abbreviate the word editors as “Eds.” instead of “Ed.”

Academic theses:

[1] A. Student, PhD thesis, University of Zurich (Switzerland), **1991**.

Software:

The author guidelines of Angewandte Chemie International Edition suggest to cite software directly:

[1] G. M. Sheldrick, SHELXS–96, Program for the Solution of Crystal Structures, University of Göttingen, Göttingen (Germany), **1996**.

However, the problem of citing software directly is that these citations are not counted towards the many indices that rely on citation counting (*cf.* section 2.2.2). Therefore, check whether you can cite an article in a scientific journal that describes the software. In the case of the example above this could be

[1] G. M. Sheldrick, *Acta Crystallogr., Sect. A: Found. Adv.* **2008**, *64*, 112–122.

Manuals of practical courses:

[1] Practical Course in Biochemistry, Manual, University of Zurich, **2016**.

Currently, there are no generally accepted standards how to cite online sources as already discussed in section 2.2.2. Therefore, the author guidelines of *Angewandte Chemie International Edition* (this is similar for other journals) provide just one example that seems to be insufficient. Consider the following examples and the citations in chapter 6[1–3,18–20] as recommendation how to cite online sources. Because of the lacking standards, handling citations of online sources by citation management programs may also not be straightforward.

Entries in online databases:

[1] J. Hartmann-Schreyer in *Roempp Online*, entry *Salzsäure*, Thieme, Stuttgart, **2004**; retrieved 18. Aug. 2016 from http://roempp.thieme.de.[1]
[2] O. Nuyken, H. Samarian, C. Nagel-Ogric in *ChemgaPedia*, entry *Kautschuk*, Wiley Information Services GmbH, Berlin; retrieved 19. Aug. 2016 from http://www.chemgapedia.de/vsengine/vlu/vsc/de/ch/9/mac/andere/kautschuk/kautschuk.vlu.html.[2]

Online database in general:

[1] *NIST Chemistry WebBook*, National Institute of Standards and Technology, Gaithersburg, **2016**; retrieved 19. Aug. 2016 from http://webbook.nist.gov/chemistry/.

Electronic book:

[1] F.L. Hitchcock, C.S. Robinson, *Differential Equations in Applied Chemistry*, John Wiley & Sons, New York, **1923**; retrieved 19. Aug. 2016 as ebook from https://archive.org/details/differentialequa031879mbp.

4.6 Text

4.6.1 Active or Passive Voice

Active voice is attractive to read. This may help to present science in an appealing way to a wider audience especially outside science. Actually, many scientific journals prefer active voice. However, active voice directs the focus on the *person* who did something. Therefore, active voice may be enticing to report in a less neutral way. Passive voice directs the focus on *what* that person did. The latter seems to be more appropriate for a scientific report. Passive voice is considered neutral, reserved, and objective.

Therefore, we recommend that you use passive voice in your laboratory reports. This is especially true for the experimental part. Write “Compound **1** (10 mg) were dissolved in ethanol (100 mL)” instead of “I (or we) dissolved compound **1** (10 mg) …”

Avoid switching from passive to active voice and *vice versa* unnecessarily. However, you may change the voice as a stylistic means to distinguish paragraphs with a different purpose. For example, you can clearly separate experimental facts (passive voice) from your interpretation or suggestions (active voice). “It is concluded …” sounds strict and non-negotiable whereas “We conclude …” leaves more space for alternatives.

4.6.2 Tense

You performed your experiments in the past. Therefore, the only natural choice for the tense of your report is the past tense. Use the past tense to describe your experiments and your

[1] Note that 2004 refers to the date of the last modification of the entry *Salzsäure*.
[2] No information on the date of the last modification is available.

experimental results. The past tense is also appropriate for a summary of what other researchers found or for a historical review. Use the simple past tense for finished actions that occurred at a specific time in the past. Use the present perfect tense for actions which started in the past but are still ongoing or when the effect of a past action continues to be important in the present.

Your report will contain many general statements, *e.g.* “The *Hagen–Poiseuille* equation describes the flow through a capillary” or “Fig. 2 shows the IR spectra”. These statements are valid independent of time. Therefore, use the present tense. It is also a good idea to use the present tense for your interpretations or conclusions. This helps to distinguish experimental facts from potentially less safe conjectures.

You should use the subjunctive to mark your statement clearly as an unproven idea or speculation. Speculating is allowed but should be in reasonable proportion to facts.

Do not switch tenses unnecessarily.

4.6.3 Writing Style

Writing style is a very difficult topic for several reasons. There is no clear definition of a good or bad writing style. It is largely a matter of personal perception or taste. In addition, the scientific *lingua franca* is English. English is not the mother tongue for most scientists and students at the University of Zurich (including the authors of this handbook). Thus, writing in a good style is difficult and teaching good style is even more difficult. Correcting written reports with respect to style is almost impossible for young and unexperienced teaching assistants.

Scientifically correct presentation of your experiments and results is most important for your laboratory reports during the first laboratory courses. For these reasons, we keep this section short and provide only very few general rules. We encourage you to consult the recommended literature.[21,20]

- Use either American or British spelling. Do not mix both spellings.
- Correct grammar is a must.
- Try to write in short, simple, and complete sentences. The subject should be located close to the verb. Avoid complex structures that are often used in written German.
- Do not start sentences with “but”, “and”, “because”, and “so”. Use appropriate linking words instead. Do not end sentences with “too”, “also”, “though”, or “yet”.
- Avoid the verb “get” in written English.
- “This” and “these” are unclear references if not followed by a noun. “This was an unexpected result” is worse than “This result was unexpected”.
- Deal with only one topic per paragraph. Use one introductory sentence and then develop the topic.
- Use only complete comparisons. “The yield was lower.” is not very helpful. Lower than what? A better variant is: “The yield in ethanol as solvent was lower by a factor of two compared to methanol.”
- Avoid empty or needless words or phrases. Examples are:
  “The sample was treated with a solvent”. What does treated mean? Replace “treated” by “immersed, washed, dissolved in” or whatever is appropriate or more precise.
  “We used high-quality products”. A better choice is “products with high purity” or “products according to DIN ISO xxx”.
  “The yield is low”. How much is low? Provide numbers or comparisons to other values.

- Simplify unnecessarily lengthy expressions. Examples: “due to the fact that” or “owing to the fact that” are both identical to “because”; “circular in shape” means “circular”; replace “if conditions are such that” by “if”.
- Avoid the gerund of verbs to create nouns when a good noun exists. “(By) using water” is not incorrect but may be too colloquial. “By the use of water” is more formal.
- Try to link successive sentences, paragraphs, and sections. Linking can be achieved by “linking words” (however, since then, in addition, therefore, thus, hence, nevertheless, in contrast, otherwise …). You can also repeat important phrases: “It is known that the addition of formic acid enhances the *catalytic activity* of ruthenium complexes. According to our results, the *catalytic activity* is …”
- Try to link the discussion of the results to the introduction. If you state a hypothesis in the introduction, repeat this hypothesis by use of the same words and combine it with your results.

4.6.4 Fonts

It is tempting to play with less usual fonts when writing your first reports. Use only standard fonts for the sake of good legibility. First, less common fonts may not be installed on other computers or other operating systems. Thus, they may not reproduce as intended when you exchange files. Second, our brain recognises words (or parts of lengthy words) just as it recognises images. As you recognise your parents on a photograph within fractions of a second, your brain recognises the written words of this text as a whole while you read it. This works the better and makes reading faster, the more your brain is familiar with the font. Do not use strange fonts because the reader has to decipher the text letter by letter very slowly. Fonts with serifs are most appropriate for normal text (*e.g. Times New Roman*). For labels, graphs, artwork, or possibly headlines, fonts without serifs are a good choice. Prefer *Helvetica* or *Arial*.

It is common to use the font *Symbol* for Greek letters. However, the typeface of *Symbol* rarely matches the typeface of the font that you use for normal text. This is especially true for fonts without serifs. Compare the combination of *Symbol* and *Arial* in µm and plain *Arial* in µm. Using the Greek letters of your standard font instead of *Symbol* offers the big advantage that you do not have to switch fonts before and after any Greek character. On the other hand, finding and inserting the Greek letter of a normal font may also be awkward. Whichever way you chose, use shortcuts or the AutoCorrect function (*cf.* sections 5.4 and 5.5) to simplify the selection of fonts and the insertion of special characters.

It is common in scientific literature to italicise proper names and Latin or Greek loanwords or abbreviations. Write *A. Einstein*, *Fehling’s* reagent, *e.g.*, *et al.*, *i.e.*, and *in situ*.

A confusing issue is when to use the hyphen “-“, the en-dash “–“ (also N-dash because its length corresponds to the width of a capital N), or the em-dash “—“ (also M-dash because its length corresponds to the width of a capital M). Use the en-dash for linking two words of equal rank (“solid–liquid”), for linking two names (“*Diels–Alder* reaction”), for indicating a range of values when space is limited (“2 m – 4 m” instead of “from 2 m to 4 m”), or for page ranges (“pp. 113–120”). Use the em-dash to separate a less important part of a sentence similar to the usage of parentheses. Do not use blanks with em-dashes: “The sky is—as anyone would expect—blue.”. The rules for hyphenation are too numerous to be listed here.[20] A coarse approximation is to use hyphens when the rules for en-dashes or em-dashes do not apply. Use the true minus sign “−” in mathematical expressions (*cf.* section 4.1).

5 Efficient Use of a Word Processor

Conducting scientific experiments and reporting them is mentally taxing. Therefore, save your mental capacities for the creative part of this work and delegate monotonous and recurring jobs to your computer. It is designed for such work. The crux of this matter is, that figuring out how to "tell" your computer what you would like it to do is often time-consuming, laborious, or even impossible without professional help. Even advanced users are simply not aware of all the possibilities their software may offer. Therefore, especially for beginners, it often seems to be faster to do all the work by hand. This may even be true for comparatively short laboratory reports with two figures and three citations, for example. However, numbering figures and cross-references by hand, formatting text with blanks, tabs and line breaks, and finally adding a table of contents by hand is excessively arduous, time-consuming, and prone to errors. All of these problems are critical to academic theses, which are often generated under time pressure, may contain hundreds of numbered items and several tens of different formatting styles, and which should convey exactness in their optical appearance.

The following sections 5.1 to 5.5 intend to make you aware of important features of a word processor. Any further introduction to word processors exceeds the idea of this handbook. We strongly recommend that you use these features and that you exercise how to use your word processor efficiently from the beginning. Only then, you are prepared to handle a master thesis or PhD thesis efficiently. Many students underestimate the time that is necessary for the final layout and formatting of a thesis. We also recommend attending the courses that are offered by the Informatikdienste of the University of Zurich.

5.1 Automatic Numbering

A report contains many components that have to be numbered consecutively. These components are chapters, chemical compounds, figures, tables, or equations to name only a few. Use the automatic numbering feature of your word processor wherever possible. It guarantees that your numbers are consecutive and unique. You can trigger an automatic update of the numbering when the sequence of *e.g.* figures has to be changed or figures have to be removed or added. Such changes are frequent! Apart from number ranges, which are pre-defined in your word processor, you can define your own number ranges. Do not use the end-note feature (the one which is built in in your word processor, the external citation management software *Endnote* may be used) to number your citations. Use citation management software instead (*cf.* section 4.5.2).

5.1.1 Cross-References

A further and major advantage of automatic numbering is that you can create cross-references to automatically numbered items. These cross-references also updated as soon as the numbering for the original items changes. This is a very powerful tool because every numbered item has to be referred to at least once in a scientific report. Unfortunately, this feature is incompletely implemented in the most common word processor *MS Word*. Inserting cross-references to chapter numbers or page numbers works. Inserting cross-references to number ranges defined by the user does not work reliably! Inserting cross-references to pre-defined number ranges works but there are no further options with regard to formatting or other necessary adaptations, which renders this option almost useless. Alternatively, you can use a system of unique wild cards, *e.g.* f$001, f$002 … for the numbers of figures and corresponding cross-references. After all editing is finished and the final sequence is fixed, replace all wild cards by the final number. However, this requires several rounds of search and replace!

5.1.2 Automatically Generated Lists

You can easily create a formatted list of automatically numbered items. Generating a table of contents from automatically assigned chapter numbers and chapter headings is timesaving. For a master or PhD thesis or a review article, automatically generated lists of figures or tables are very helpful.

5.1.3 Footnotes

Any word processor offers to insert automatically numbered footnotes. You may use this option in laboratory reports for side remarks. Do not use the endnote feature of your word processor.

5.2 Style Sheets

A very important and underestimated tool is the use of style sheets. Style sheets can ease the work of formatting substantially. You can use a pre-defined style sheet or define a new style sheet according to your needs. Style sheets exist for nearly anything that can be formatted. They are especially useful for the consistent formatting of chapter headings, tables, images, or figure captions. The possibilities are too numerous to be listed here. The formatting of a line containing a formula may serve as an example:

$$a^2 + b^2 = c^2. \tag{2}$$

The formatting of this single line as paragraph needs a centred tabulator at 8 cm (centre of the page) for the formula and a tabulator with right justification at 16 cm (at the right margin) for the number of the equation. To increase the visibility of the line, additional space above and below the paragraph was added. This avoids the use of additional line breaks. Once the formatting is finished, you can use this line as a template to create a new style “equation line”, for example. To format any subsequent formulae in your text exactly like the first one, simply assign your style sheet “equation line” to the corresponding paragraph. Note that you could apply the same style sheet to lines with a chemical equation instead of a mathematical one.

A further advantage of style sheets is that you can modify the format of—following the example above—all lines with an equation in your text at once simply by adapting the settings in the style sheet “equation line”.

5.3 Search and Replace

The function “search and replace” is well known. Use the full power of this feature by including styles, wild cards, and special characters for the search expression and for the replacement expression.

5.4 Auto-Correct or Auto-Replace

Chemical documents contain many symbols and characters that are not directly accessible via the keyboard. The auto-correct or auto-replace functionality of a word processor is a powerful tool to insert these characters with little effort. Nearly all word processors have a built-in list of special characters that are inserted by typing a corresponding sequence of characters (*e.g.* the arrow → can be inserted by typing the characters -->, the Greek letter Σ can be inserted by typing :Sigma:). It is very helpful to extend or modify the built-in list, especially for frequent symbols such as Greek letters, arrows, mathematical symbols, or other special characters such as Å, − (true minus), – (en-dash), — (em-dash), *ħ*, M, or †.

5.5 Shortcuts and Macros

Working with a word processor requires typing at the keyboard and using the mouse. It seems to be convenient to use the keyboard for not much more than entering text and to use the mouse for placing the cursor or navigating through menus. However, keyboard shortcuts are much faster than using the mouse. Although it might be arduous in the beginning to learn all necessary shortcuts, shortcuts save time on a long-term basis. A shortcut exists for nearly every command. Very helpful are keyboard shortcuts for frequently used fonts (*e.g. Arial*, *Times New Roman*, and *Symbol*) and type styles (*e.g.* *x*, **x**, $_{x}$, and ^{x}). If you feel a shortcut is too complicated or hard to memorise, you can define your own shortcuts according to your needs.

A more sophisticated version of processing several shortcuts in a sequence are macros. You can define your own macros to avoid the repetition of the same sequence of commands repeatedly. For example, the first words up to the first full stop in a figure caption are often printed in bold face. You could do this manually—and for all figure captions individually—by searching for the first full stop in the caption, marking all characters including the full stop to the beginning of the paragraph and then choosing boldface by hand. Alternatively, while doing this procedure once you could record the above steps with the macro recorder of your word processor. Next, assign a shortcut to the macro and start the macro in every caption.

6 References

[1] *Ethical Principles*, University of Zurich, **2015**; retrieved 03. Aug. 2016 from http://www.researchers.uzh.ch/en/ethics.html.

[2] *Wissenschaftliche Integrität. Grundsätze und Verfahrensregeln*, Swiss Academies of Arts and Sciences, **2008**; retrieved 22. Aug. 2016 from http://www.akademien-schweiz.ch/dms/D/Portrait/Kommissionen/Integritaet/Integritaet_d.pdf.

[3] *Sicherung guter wissenschaftlicher Praxis*, Deutsche Forschungsgemeinschaft, **2013**; retrieved 22. Aug. 2016 from http://www.dfg.de/download/pdf/dfg_im_profil/reden_stellungnahmen/download/empfehlung_wiss_praxis_1310.pdf.

[4] W. F. van Gunsteren, *Angew. Chem.* **2013**, *125*, 128–132.

[5] U. Böhme, S. Tesch, *Nachr. Chem.* **2014**, *62*, 852–857.

[6] U. Böhme, S. Tesch, *Nachr. Chem.* **2013**, *61*, 1230–1233.

[7] U. Böhme, S. Tesch, *Nachr. Chem.* **2016**, *64*, 992–994.

[8] E. Leusmann, C. Remenyi, *Nachr. Chem.* **2016**, *64*, 883–884.

[9] M. D. Mandler, *J. Chem. Educ.* **2017**, *94*, 271–272.

[10] a) P. Kamat, G. C. Schatz, *J. Phys. Chem. Lett.* **2014**, *5*, 1241–1242; b) J. Reedijk, *Angew. Chem.* **2012**, *124*, 852–854.

[11] G. M. Whitesides, *Adv. Mater.* **2004**, *16*, 1375–1377.

[12] *PTB-Mitt.* **2007**, *117*.

[13] *Quantities, Units, and Symbols in Physical Chemistry* (Ed.: International Union of Pure and Applied Chemistry), 3. ed., RSC Publishing, **2007**.

[14] M. Rolandi, K. Cheng, S. Pérez-Kriz, *Adv. Mater.* **2011**, *23*, 4343–4346.

[15] B. Kulamer in *The ACS style guide* (Eds.: A. M. Coghill, L. R. Garson), 3. ed., The American Chemical Society, Washington DC, **2006**, pp. 343–367.
[16] S. Bienz, L. Bigler, T. Fox, H. Meier, *Hesse–Meier–Zeeh, Spektroskopische Methoden in der organischen Chemie*, 9. ed., Georg Thieme, Stuttgart, **2016**.
[17] J. D. Watson, F. H. C. Crick, *Nature* **1953**, *171*, 737–738.
[18] *General Information on Angewandte Chemie and Author Guidelines*, Wiley-VCH, **2020**; retrieved 24. Aug. 2020 from https://onlinelibrary.wiley.com/page/journal/15213773/homepage/notice-to-authors.
[19] *CAS Source Index (CASSI) Search Tool*, The American Chemical Society, **2016**; retrieved 22. Feb. 2016 from http://cassi.cas.org/search.jsp.
[20] *Scientific Style and Format Online*, The Council of Science Editors, **2014**; retrieved 02. Aug. 2016 from http://www.scientificstyleandformat.org/Home.html.
[21] T. Skern, *Writing Scientific English*. *A workbook*, 2. ed., Facultas, Wien, **2011**.