

Science of Synthesis

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Preface

Science of Synthesis

Science of Synthesis was launched in 2000 and was initially edited by D. Bellus (Basel, Switzerland), E. N. Jacobsen (Cambridge, USA), S. V. Ley (Cambridge, UK), R. Noyori (Nagoya, Japan), M. Regitz (Kaiserslautern, Germany), P. J. Reider (Princeton, USA), E. Schaumann (Clausthal-Zellerfeld, Germany), I. Shinkai (Tokyo, Japan), E. J. Thomas (Manchester, UK), and B. M. Trost (Stanford, USA). *Science of Synthesis* is a balanced and critical reference work produced by the collaborative efforts of chemists, from both industry and academia, selected by the Editorial Board. All published results from journals, books, and patent literature from the early 1800s until the year of publication are considered by the authors, who are among the leading experts in their field, to provide chemists with the most reliable methods to solve their synthesis problems.

Science of Synthesis is organized in a logical hierarchical system based on the target molecule to be synthesized. The critical coverage of methods is supported by information intended to help the user choose the most suitable method for their application, thus providing a strong foundation from which to develop a successful synthetic route. Within each category of product, illuminating background information such as history, nomenclature, structure, stability, reactivity, properties, safety, and environmental aspects are discussed along with a detailed selection of reliable methods. Each method and variation is accompanied by reaction schemes, tables of examples, experimental procedures, and a background discussion of mechanistic rationale, stereochemistry, scope of the reaction described and its limitations, and functional group compatibility. In a format consisting of 48 volumes, *Science of Synthesis* is a unique reference work, selecting and evaluating all synthetic methodology and thus providing more than just a compound database or an indiscriminate review of the literature.

Science of Synthesis Knowledge Updates

From 2010 onwards, the organic chemistry reference series *Science of Synthesis* has been continuously updated with high-quality content using clearly defined criteria for method selection as well as established editorial processes. The Editorial Board, in conjunction with selected volume editors and authors, are reviewing the whole field of synthetic organic chemistry as presented in *Science of Synthesis* and are evaluating significant developments in synthetic methodology.

The series is currently edited by E. M. Carreira (Zurich, Switzerland), M. Faul (Thousand Oaks, USA), S. Kobayashi (Tokyo, Japan), G. Koch (Schlieren, Switzerland), C. Nevado (Zurich, Switzerland), D. Sarlah (Texas, USA), T. P. Yoon, (Wisconsin, USA), and S.-L. You (Shanghai, China).

A list of criteria for method selection guides the updating process in order to guarantee that only the best and most reliable synthetic methods are included in *Science of Synthesis*. Authors involved in the updating process add new methods and add new (or completely revise existing) product (sub)classes.

The updating procedure is continuous and new content is added to the electronic version in four releases per year. *Science of Synthesis* continues to be the most up-to-date evaluated electronic reference work available, emphasizing the most significant developments in synthetic methodology.

Science of Synthesis gives convenient access to a century of synthetic organic chemistry starting with the first volume of *Houben–Weyl* published in 1909 right through to groundbreaking methodology added immediately upon validation by experts. The electronic version's intuitive interface will adapt in keeping with the latest technological developments and will enable chemists worldwide in both academia and industry to solve complex synthetic problems.

Science of Synthesis Reference Library

The organic chemistry reference work *Science of Synthesis* is complemented by a series of organic synthesis specialist topic reference volumes which constitute the *Science of Synthesis* Reference Library. A modular approach is used to build the reference library, with new volumes focusing on areas of great current interest.

Whereas the *Science of Synthesis* is organized by product topology, the *Science of Synthesis* Reference Library is designed so that where possible it incorporates reaction type or technique. This additional content is complementary to the existing scaffold of core synthetic methodology available.

The *Science of Synthesis* Reference Library is developed in collaboration with members of the *Science of Synthesis* Editorial Board who help with the identification and selection of topics as well as providing guidance in relation to the scientific content and format of presentation of the product. World renowned experts are chosen as volume editors and authors of the contributions. The high editorial quality standards associated with *Science of Synthesis* are maintained and the product is made available in various digital and online formats.

The Publisher

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1 Science of Synthesis Knowledge Updates

1.1 Concept

Science of Synthesis is a reference work with the largest collection of evaluated methods in organic synthesis worldwide. This vast amount of useful organic synthetic information, which has been evaluated by leading world experts, has been available both in print and online formats. The online version of *Science of Synthesis* enables text, structure, substructure, and reaction searching via a simple interface with powerful functionality. Continual updating of the electronic version means that the content of *Science of Synthesis* remains pertinent and relevant to the synthetic organic chemist's needs. Also, supplementing current content with special topics (e.g., catalytic stereoselective synthesis, photocatalysis, flow chemistry, etc.) acknowledges the broad spectrum of organic chemistry today and the need for chemists to appreciate many different peripheral scientific fields in addition to the core subject area.

Three types of update are published in Science of Synthesis Knowledge Updates:

- **revised product classes/subclasses**, i.e. complete revision of entire contributions
- **addition of product classes/subclasses**, i.e. the addition of entirely new contributions
- **addition of methods to product classes/subclasses**, i.e. supplementary material

To ensure that users also have access to the most interesting and recent trends in synthetic chemistry, there will be links in place from Science of Synthesis contributions to other relevant content via the Thieme Chemistry discovery platform SynOne.

1.2 Objectives, Scope, and Selection Criteria

The **title**, **subject**, and **scope** of the assigned contribution are to be clarified with the volume editor.

The aim of Science of Synthesis is to provide the readers with a **critical review** of the methodology chosen and to present the contribution in an informative and readable style. Wherever possible, the author should **compare and contrast similar methods/variations and point out the advantages and disadvantages** of the various approaches.

Structure/Table of Contents: If the contribution is a revision or the addition of supplementary material, it is advisable that the author uses the original contribution as a basis for the structure of the chapter. If the author wishes to adopt a significantly different structure for the update, the volume editor and editorial office should be consulted. For new product classes/subclasses, the author should look at the general structure of related chapters in SOS and should base the structure of their chapter on these. It is recommended that once the author has a rough plan for the structure of the the update chapter, a provisional table of contents is submitted to the volume editor and editorial office for review.

Access to the electronic version of Science of Synthesis is provided to all authors during the period of writing to assist with decisions regarding content and style.

Science of Synthesis Knowledge Updates critically evaluate the methods that are of most significance for modern organic synthesis. *Science of Synthesis* is oriented toward synthesis and the selection of the best and most reliable synthetic procedures. In particular, all synthetic methodology reported should be checked for:

- ease of execution
- scope
- yield
- cost
- environmental issues
- are there easier/better methods available?

A reaction can be of high mechanistic and theoretical interest, but this is not a sufficient criterion for inclusion in *Science of Synthesis*. A synthetic method may be very interesting from the point of view of the mechanism, but if there is an easier and less expensive alternative then only this will be reported in detail. The interesting alternative may or may not be mentioned in passing.

Authors are encouraged to report synthetic methods which would typically have been successfully applied to six different compounds with good yields. Methods that have only been reported for two or three compounds with varying yields need to be further evaluated.

For all methods, references to the pertinent literature should be given. Important references to a particular procedure should also be given.

Books, journals, and the patent literature should be considered equally. References to patents should be given whenever they contain relevant information.

Science of Synthesis Knowledge Updates is oriented toward synthesis and, whilst the exact nature of the chapter will determine its content, the focus should be on the application of reactions/techniques/apparatus in synthetic organic chemistry and the selection of the best and most reliable synthetic procedures. Comments should be made on the synthetic importance of the approach, the ease of execution, the yield of reaction, the cost of the reaction, and green issues.

A typical manuscript covering the synthesis of a product (sub)class would contain the elements below. However, if the chapter is a “supplementary” update, the background information does not need to be repeated. Instead, a brief introduction, placing the new/improved methods in context with the methods reported in the original *Science of Synthesis* review should be provided.

- Product (Sub)Class/es:
- Background Information
 - History
 - Nomenclature
 - Important Applications
 - Structure
 - Stability
 - Reactivity
 - Physical Properties
 - Spectroscopic Properties
 - Safety and Environmental Aspects
- Method/s for Synthesis:
 - Details of Method
 - Comparison/Contrasting of Methods
 - Robustness, Limitations and Problems
 - Scalability
 - Safety and Environmental Aspects
 - Mechanistic Rationale
 - Stereochemistry
 - Scope (illustrated with tables of examples)
 - Functional-Group Compatibility
 - Discussion of Variations on the Method
 - Scheme(s) and Tables of Examples
 - Experimental Procedure/s (past tense and labeled as General or Typical if necessary)
- References

2 Manuscript Preparation

Authors will be given full access to the online version of Science of Synthesis for the duration of the writing process. It is strongly recommended that authors look at existing chapters to familiarize themselves with the general style and presentation used in Science of Synthesis. A sample contribution will also be sent to all authors to help as a guide regarding the styles and conventions used in *Science of Synthesis*.

All parts of *Science of Synthesis* will be written in American English. All parts of the manuscript should be written in the present or relevant tense, except for the experimental procedures, which should be written in the past tense.

At an early stage in the writing process, authors are encouraged to send a few **sample pages** to the editorial office, which will provide feedback.

The division of a chapter into subsections is at the discretion of the author, subject to the approval of the volume editor. However, no more than six hierarchical levels of subsections should be used.

2.1 Manuscript Length

Authors are requested not to exceed the given number of typeset pages for their manuscript. If during the writing process author realize their manuscripts will differ significantly from the agreed length, they are asked to contact the volume editor and the editorial office as soon as possible.

For estimating the final length of a contribution, the following general rules should be used (assuming that the author has used the document template):

1 typeset page = 2 Microsoft Word pages (without graphics pasted in)

1 typeset page = 1½ Microsoft Word pages (with graphics pasted into the Word document)

2.2 Use of the Document Template

Authors will be sent a style template for Microsoft Word (scisynth.dot). The template is also available to download from the *Science of Synthesis* website. The *Science of Synthesis* document template contains a list of formatting styles that should be applied to the various titles in the manuscript. Unlike the templates for many journal submissions, the layout and appearance of your manuscript in the template will look very different to the final typeset manuscript (you will see the layout when you receive the [page proofs](#)). A sample chapter, as it appears when using the template, is also included in the author pack. This file (SampChap.doc) is intended to illustrate how the template should be used and the various styles should be applied.

2.3 Guidelines for Text

2.3.1 Format of Text

The text should be prepared using the *Science of Synthesis* document template. Underlining, indentations, and block capitals should be avoided. Boldface and italic fonts should be used according to the instructions [e.g., amine **6**; *J. Org. Chem.*, (1973) **38**, 3438]. References should be included at the end of the manuscript. Tables should be included in the appropriate position in the body of the text. Tables, schemes, formulas for tables, and figures should be numbered with Arabic numbers, not Roman numerals.

2.3.2 Writing Style

- Use American spelling.
- All parts of the manuscript should be written in the **present** or **relevant** tense, except for the **experimental procedures**, which should be written in the **past** tense.
- For style of the manuscripts the ACS Style Guide [*The ACS Style Guide*, 3rd ed.; Coghill, A. M.; Garson, L. R., Eds.; Oxford University Press: New York, (2006)] should be consulted.
- **Compound numbers** should only be used if the compound is referred to in the text. It is not necessary to number every compound. Where the full name of a compound is given, the compound number should appear emboldened in parentheses [e.g., (S)-butan-2-ol (**23**)]. If the full name is not given then the number simply appears in bold, no parentheses (e.g., alcohol **23**).

2.3.3 Nomenclature

In general, and in particular for the naming of specific compounds that are the titles of experimental procedures, *Science of Synthesis* uses nomenclature **based on the rules of IUPAC**. An exception is the naming of ring systems, whose names and numberings may be taken or derived from the *Ring Systems Handbook* [American Chemical Society: Columbus OH, (1988) and supplements]. Trivial names should be avoided unless they offer a distinct advantage over the corresponding systematic name or are much more commonly used than the IUPAC name. For classes of complex natural compounds, such as carbohydrates, peptides, or steroids, the most common name should be given. Compounds which are not named or have long names should be referred to unambiguously as “amine **2**” or “thioester **14**”.

2.3.4 Units

- For pressure, Torr, atm, or Pa are recommended [note: 1013.25 mbar = 760 Torr = 101325 Pa = 14.696 psi].
- For temperature, use °C. For very low temperatures, K is also acceptable.
- Metric units (SI) should be used in all other cases, although the unit kcal will also be accepted.

2.3.5 Abbreviations

- Abbreviations and simple chemical formulas (e.g., CH₂Cl₂) should be used in tables, schemes, and experimental procedures.
- Avoid abbreviations/chemical formulas in titles and the discussion text (e.g., CO should read carbon monoxide).
- Common abbreviations used in *Science of Synthesis* are available [here](#).
- Abbreviations for journal titles are available [here](#).

2.3.6 Experimental Procedures

- Experimental procedures should follow the style of the Thieme journal **SYNTHESIS**.
- The experimental procedure itself is entitled with the product, or general classification of the product name, followed by the compound number.
- All experimental procedures should be classified as one of the following:
 1. General Procedure: A generalized version of a widely applicable experimental procedure.
 2. Typical Procedure: A specific example of a widely applicable experimental procedure.
 3. Single Procedure: Single procedures are not to be labeled as such, but are defined as follows: A specific experimental procedure for a single compound which is not applicable to similar compounds or for which the scope has not been studied.

As the criteria used to assess methods for inclusion in Science of Synthesis include range of applicability, the majority of procedures will be Typical or General Procedures; non-typical procedures for individual examples are restricted to unique methods that are particularly useful for the synthesis of one synthetically important compound or intermediate.

- All titles of experimental procedures should have a reference citation.
- The author should indicate aspects of the procedure which are particularly critical to success, including any new observations on or adaptations of older literature methods.
- Available details of workup should be included.
- Physical or spectroscopic data should be given only to a very limited extent.
- The slash symbol is to be used for (1) surfaces, e.g. Pd/C; (2) alloys and amalgams, e.g. 5% Na/Hg, Na/K (1:1); (3) solvent mixtures, e.g. EtOH/MeOH (95:5); (4) reagent concentrations, e.g. 2% HCl/H₂O; (5) single reagents, e.g. Li/NH₃.

- Write procedures in the **past** tense and include the mass, number of moles, volume, etc., in brackets **after** the name of the substances or solvents.
- Avoid starting sentences with numbers, wherever possible.
- Procedures from preparative book series, such as *Organic Syntheses* are **not allowed** for reproduction. If necessary, a short comment on relevant procedures of the same type should be made.

Example Experimental Procedure

Tributyl[(2*R*)-3-(methoxymethoxy)-2-methylpropyl]stannane (**4**); Typical Procedure:^[25]

CAUTION: *Technical grade chloromethyl methyl ether is classified as a human carcinogen, and is an eye and respiratory tract irritant.*

A soln of crude **3** (7.3 g, from 15 mmol of **2**) in THF (40 mL) was cooled in an ice bath and NaOH (1.5 g, 37 mmol) in H₂O (8 mL) was added, followed by dropwise addition of 30% H₂O₂ (5 mL, 50 mmol). The mixture was kept at 0 °C for 1 h, and then at 25 °C for 6 h, during which time a pasty, colorless precipitate formed. The mixture was treated with Et₂O (50 mL) and filtered. The aqueous phase was separated and extracted with Et₂O (3 × 30 mL) and the combined organic phase was dried (MgSO₄) and concentrated. The gel-like residue was flash chromatographed [silica gel, petroleum ether (bp 30–40 °C)/Et₂O 9:1] to give the labile intermediate; yield: 3.98 g (76%); this was reacted further without characterization. To a soln of the intermediate (3.6 g, 10 mmol) in CH₂Cl₂ (10 mL) was added iPr₂NEt (1.2 g, 10 mmol), followed by MOMCl (0.89 g, 11 mmol). The mixture was stirred for 1 h at 0 °C and 15 h at 25 °C, and then concentrated. The resultant residue was treated with ice-cold 2 M HCl (10 mL) and extracted with petroleum ether (bp 30–40 °C; 2 × 20 mL). Concentration of the organic phase (10 Pa) gave the product as a colorless solid; yield: 3.7 g (92%); mp 130 °C.

2.3.7 Safety and Environmental Aspects

Chemicals are associated with two types of hazard: hazards that are a direct result of the physical or reactive properties of a chemical; and hazards posed by the effect of a chemical on biological systems. Flammability and the stability of a chemical in air or toward water may be included in the first group, while the carcinogenic potential of a chemical or its effect on the reproductive system are health hazards due to the biological properties of a chemical. The different hazardous properties that authors should take into consideration when evaluating experimental procedures are as follows:

Physical and reactive chemical hazards:

- Flammability and explosive properties
- Stability in air or in contact with water (pyrophoric and water-reactive compounds)
- Incompatibility with commonly available chemicals and reagents

- Potential for peroxidation
- Oxidizing or reducing properties
- Storage properties

Health effects of chemicals:

- Known human carcinogens and probable human carcinogens according to the International Agency for Research on Cancer (IARC) classifications
- Known human teratogens and chemicals known to have an effect on human reproduction
- Chemicals that are irritants to the skin, eyes, or respiratory system (data from human exposure/animal tests)
- Chemicals that are corrosive to the skin, eyes, or respiratory system (data from human exposure/ animal tests)
- Skin sensitizers
- Chemicals that are highly toxic as a result of some specific pharmacological mechanism (e.g., the potent neurotoxin tetrodotoxin)

It is important that authors discuss potential hazards of the described compounds. Furthermore, the methods described in *Science of Synthesis* should be discussed in terms of atom economy, as well as their possible impact on the environment. If toxic solvents (e.g., chloroform), toxic catalysts [e.g., mercury(II) chloride], toxic reagents (e.g., phosgene), or any other hazardous compounds are used or recommended in certain experimental procedures, alternatives should be discussed. Safety guidelines should be given for dangerous compounds or procedures. Warnings in experimental procedures should be given using the following format:

CAUTION: *Hexamethyltungsten(VI) is known to decompose explosively. Proper safety precautions should be taken during its synthesis, storage, and handling.*

2.3.8 Copyright

It is the responsibility of the author to obtain, where necessary, copyright permission for figures (see [Section 2.5.3](#)), tables, schemes, or textual information from another source that is to be reproduced in a *Science of Synthesis* contribution. The editorial office can always be contacted for advice on such matters, and will help authors to direct applications to the appropriate departments. In the case of reproduction of experimental procedures and schemes from journal publications, a full citation in the references section is sufficient acknowledgement of copyright

ownership. Problems concerning copyright infringement usually arise when text or figures are taken from books [e.g., Brandsma, L.; Verkruijsse, H. D., *Synthesis of Allenes and Cumulenes*, Elsevier: Amsterdam, (1981)] or serial publications [e.g., *Organic Syntheses*, Coll. Vol. VI, Noland, W.E., Ed; Wiley: New York, (1988)] without significant adaptation of the original version. The copy editor assigned to each manuscript will advise the author of the need to obtain copyright, if they have not already done so, and will add the appropriate credit line. If there is an appropriate and adequate alternative to a reference requiring copyright then this reference should be substituted, or if a similar procedure is available then this procedure should be used instead of that under copyright. For any queries about copyright, please contact toby.reeve@thieme.de.

2.4 Guidelines for References and Cross-References

- References should be placed collectively at the end of the manuscript.
- References should be numbered consecutively within chapters, with no subdivisions such as ^[3a], ^[3b], ^[3c], etc.
- Each reference number should contain only one citation.
- Use one reference number for each reference only; do not repeat a reference citation with a new number every time it appears.
- References to the literature should appear in the text, tables, and scheme headings as superscript Arabic numerals in square brackets following the punctuation, e.g. This is a sample sentence.^[1]
- Authors should include reference numbers for schemes and figures in the scheme/figure titles.
- Reference numbers for tables should be included in the tables as the final column, with the heading Ref.
- *Journals*: provide the names of all authors. Do not use “et al.”. A comma should be used to separate the name of the last author and the title of the journal.
- Use the journal abbreviation in accordance with the list available [here](#). For journals not listed, please give the full journal name or the [CASSI](#) abbreviation.
- *Books*: see sample references for books with and without editor.
- *Patents*: see sample reference. Important patents should be read in the original versions as *Chemical Abstracts* reports often do not contain all important details.
- *Databases and Websites*: reference can also be given to records in databases or information on websites.
- If reference is made to a less readily available journal, the *Chemical Abstracts* reference or the English translation [e.g., *J. Gen. Chem. USSR (Engl. Transl.)*] should also be cited.
- The use of a reference-managing program (e.g., EndNote) is strongly recommended (note, however, that use of the endnote function in MS Word is *not* recommended).

Sample References

- [1] Trost, B. M.; Biddlecom, W. G., *J. Org. Chem.*, (1973) **38**, 3438.
- [2] Hoppe, D.; Gonschorrek, C.; Egert, E.; Schmidt, D., *Angew. Chem.*, (1985) **97**, 706; *Angew. Chem. Int. Ed. Engl.*, (1985) **24**, 700; footnote 12.
- [3] Pratt, A. J.; Thomas, E. J., *J. Chem. Soc., Perkin Trans. 1*, (1989), 1521.
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- [10] Alper, H., EP 305089, (1989); *Chem. Abstr.*, (1989) **112**, 76610.
- [11] Studer, A., Ph.D. Dissertation ETH Zürich, (1995), pp 3, 116; cf. ref 14.
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- [13] Smith, A. B., III; Fukui, M.; Vaccaro, H. A.; Empfield, J. R., *J. Am. Chem. Soc.*, (1991) **113**, 2071.

2.5 Guidelines for Graphics and Tables

Scheme: A graphic containing chemical structures (not only chemical reactions).

Figure: A graphic containing pictorial information such as a photograph, illustration of chemical apparatus, an NMR spectrum, a graph, or a timeline.

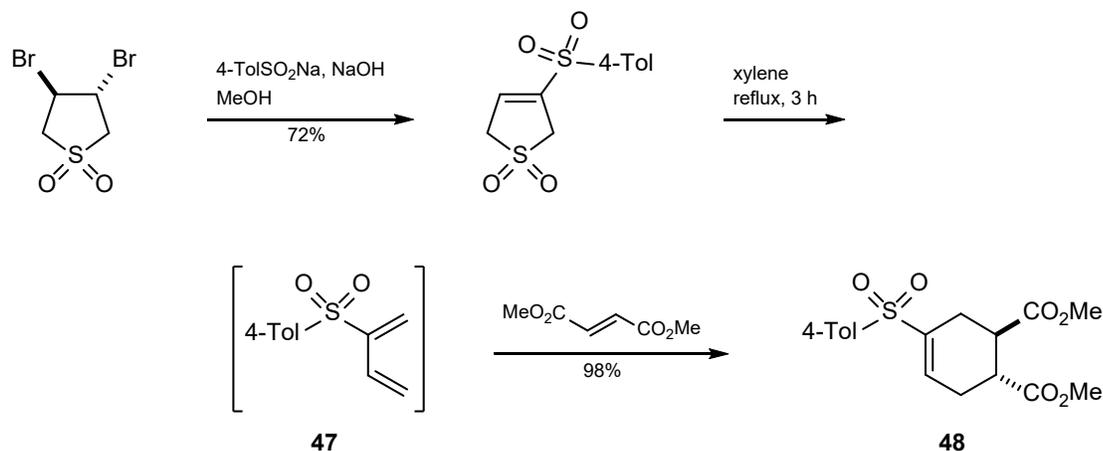
Compound numbers should only be used if the compound is referred to in the text. Not all structures need to have a compound number. Only products of experimental procedures *must* have a compound number. All compound numbers should be referred to somewhere in the text.

2.5.1 Guidelines for Schemes

- Please use the *Science of Synthesis* drawing settings that are available in ChemDraw (File -> Apply Document Settings from -> Science of Synthesis).
- The schemes should be visual abstracts of the reactions performed, hence reaction schemes are preferred to individual structures.

- Schemes should be numbered with Arabic numerals and have titles with initial letters of major words capitalized.
- When referring for the first time to information given in a scheme, please quote the scheme number in brackets.
- A scheme should be indicated in the text in the following way:

<Scheme 1> Synthesis and Reaction of a Dienyl Sulfone^[8,9]



- Schemes should *not* be electronically embedded in the text (copy/paste from ChemDraw is OK).
- Schemes should not exceed a width of 16 cm (using the *Science of Synthesis* settings in ChemDraw); schemes wider than this will need to be modified by the editorial office.
- Reaction arrows should normally be oriented horizontally, using more than one “line” if necessary. If there are still space constrictions, arrows oriented vertically or at 45° angles may be permitted. Authors should try to make efficient use of the space.
- Products of experimental procedures (and substrates and intermediates that are referred to in the text) should be numbered with bold Arabic numbers from left to right in sequence as they appear in the schemes. Begin from **1** at the start of each manuscript.
- Not every compound in a scheme needs to have a number. However, the title compound in an experimental procedure should have a number.
- For compounds with varying substituents, the labels R¹, R², X, etc. must be used and defined in a table or schemetable. Do not use R without a superscript.
- Use + and – (i.e., plus and minus symbols as superscripts) for electric charges (do not circle them).
- Two dots should be used to indicate a lone pair.

- Reagents, conditions, etc., should only appear *above* the arrow.
- Unstable/transient intermediates should be drawn in square brackets (see below).
- Each individual reagent, condition, etc., should be separated from the next by a comma and one character space, not a semicolon or solidus (forward slash); no comma should appear at the end of a line.
- Reagents, conditions, etc., appear in the following order:
 - (1) Reagents, including catalysts, e.g. H₂(g), Pd/C, Pd(PPh₃)₄.
 - (2) No. of equivalents/mol%.
 - (3) Solvents.
 - (4) Special apparatus, e.g. sealed tube, autoclave.
 - (5) Temperature, e.g. rt, 50 °C, reflux.
 - (6) Pressure, e.g. 5 atm, 100 Pa.
 - (7) Time, e.g. 5 min, 6 h, 12 d.
- Eliminated products (preceded by a minus sign) and the reaction yield appear below the arrow.
- Please do not use wedged bonds (bold or hashed) to represent chiral centers; use normal bold or hashed bonds instead.
- References will not appear in schemes but in the scheme headings.

2.5.2 Guidelines for Tables and Schemetables

All Tables and Schemetables should be constructed using the table set-up tools in Word. Please *do not* construct tables in ChemDraw.

Tables

Tables should be used to display examples of similar products prepared by a given approach in order that they may be critically discussed in the text. *Tables should show the full structure of starting materials and product in the relevant table columns. Do not list every example known;* only selected examples should be given. Tables should typically contain 5 to 10 examples and should be placed in the appropriate position in the body of the text. Tables should be numbered with Arabic numerals and have captions with initial letters of major words capitalized. When referring for the first time to information given in a table, please quote the table number in brackets. The position of a table should be indicated in the text in the way shown in the sample Table below.

In tables, collect comparable examples and quote, in the following order:

1. An entry number column may be added if this is helpful, but this is not essential
2. The starting material represented pictorially.
2. Reagents, solvents, temperature, times, as applicable.
3. Product represented pictorially.
4. ee, er, or dr when applicable.
5. Yield data.
6. Physical data, if relevant (e.g., mp).
7. Citation of the relevant literature.

Arrange the examples in a manner which best illustrates the scope and limitations of the method (e.g., they may be listed in increasing order of substituent/reagent complexity, or in increasing order of chemical or optical yield, etc.). If possible, add a generalized depiction of the reaction above the table.

<Table 1> Caption^[refs]

<Generalized depiction of the reaction>

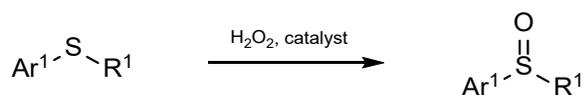
Entry	Starting Material	Reaction Conditions I	Reaction Conditions II	Product	ee or dr	Yield (%)	Ref
1	(structure)	(reagents, catalysts, solvents)	(temp, pressure, time)	(structure)			[ref no]

Schemetables

Schemetables should be employed in conjunction with schemes. They should be used to illustrate reactions when (1) there are several examples containing varying R substituents on the starting materials/products in the scheme; (2) there are different conditions (e.g., solvent, temperature, ratio of reactants) employed for the same reaction which have a significant influence on the yield, purity, or optical purity, etc. of the product.

Schemetables should be placed below the relevant scheme heading **in the body of the text**, i.e. they should be included as part of the word processor document (not in ChemDraw). Schemetables will not have a caption but should be headed **<Schemetable n>** where n is the same number as the corresponding scheme. The content and layout of a schemetable should be similar to that employed for a table, and in all cases should be kept as simple as possible. An example of a schemetable is given below:

< Scheme 12 > Oxidation of Aryl Sulfides with Hydrogen Peroxide in the Presence of Various Catalysts^[54–58]



<Schemetable 12>

Ar ¹	R	Conditions	Yield (%)	Ref
4-ClC ₆ H ₄	Me	H ₂ O ₂ , VO(acac) ₂ , EtOH, rt	90	[54,55]
Ph	Me	UHP ^a , Re(PPh ₃) ₂ OCl ₃ , MeCN	92	[56]
Ph	Ph	H ₂ O ₂ , TiCl ₃ , EtOH, rt	100	[57]
Ph	Et	H ₂ O ₂ , TeO ₂ , HCl, MeOH	92	[58]

^a UHP = urea-hydrogen peroxide adduct.

2.5.3 Guidelines for Figures

Figures should be numbered with Arabic numerals. When referring for the first time to information given in a figure, please quote the figure number in brackets. A figure should be indicated in the text in the following way:

<Figure 1> This is a Sample Figure Title^[ref]

Figures should be included in the graphics folder you submit with your manuscript. They must not be electronically embedded in the text. If possible, figures not prepared using ChemDraw should be submitted as .jpg or .tiff files, with the highest possible resolution (at least 300 dpi). As present, it is not possible to use color figures, so all figures should be black and white or greyscale.

If necessary, figures will be redrawn by the publishers and redrawn figures will be sent back to the author for checking and correction. In the case of figures taken from existing publications, it is the legal responsibility of the author to obtain permission for reproduction from the copyright holder, although the editorial office can offer assistance with such matters. Where possible this should be done at a very early stage. For figures of apparatus, please contact the apparatus producer directly. If figures are not produced by the author, the copyright of the figure must be included in the caption.

2.6 Delivery of the Manuscripts, Copyediting, and Page Proofs

2.6.1 Table of Contents

Authors are requested to send a copy of their provisional table of contents to the volume editor and to the editorial office (science-of-synthesis@thieme.de) by e-mail by the deadline specified in the Author's Agreement. Authors will then receive comments and suggestions from the volume editor and/or the editorial office.

2.6.2 Manuscript Submission

When a draft of the manuscript is complete, it should be sent by email to the volume editor(s) for review, with a copy also sent to the editorial office (science-of-synthesis@thieme.de). The volume editor will then provide feedback and may suggest changes. Once these changes have been implemented, please return the revised chapter to the volume editor for final approval.

The final manuscript, as approved by the volume editor, should be submitted to the editorial office by e-mail to: science-of-synthesis@thieme.de.

The manuscript should take the following format:

Text Folder

This folder should contain the following MS Word files

- **Abstract** consisting of 10–15 lines summarizing the content and **Keywords** (maximum 25).
- **Manuscript** with places marked for insertion of schemes, figures, and table graphics clearly labeled.

Graphics Folder

This folder should contain ChemDraw (**cdx**) files which contain the **schemes** (chemical reactions) that are to be inserted into the body of the text as well as the cdx files for any chemical structures to be drawn out in **schemetable/table entries**. Please send each scheme as a separate cdx file. Any **figures** (graphs, photographs, illustration of apparatus, etc.) should also be included as black and white (or grayscale) jpg or tiff files with the highest possible resolution. For details on the distinction between schemes, tables, and figures, please see [Sections 2.5.2](#) and [2.5.3](#).

The graphics folder should also contain a **graphical abstract**, visually summarizing the contents of the contribution with a chemical reaction scheme or illustration.

2.6.3 Copyediting Process

The manuscript submitted to the editorial office will be assigned to a copy editor who will copyedit the manuscript and apply the necessary styles for *Science of Synthesis*, e.g. check nomenclature, grammar, syntax, punctuation, phrasing, redundancy of text, and the like. The copy editor will correspond directly with authors regarding any queries and try to resolve them before proceeding to the page proof stage. If you receive a list of questions from the copyeditor, please simply answer the questions in the document you received from the copyeditor. Please *do not* send a revised version of the manuscript. However, it may be appropriate to send revised ChemDraw files if significant changes are necessary to schemes.

It is inevitable that corrections will still need to be made to the page proofs, but each copy editor will aim to eliminate as many errors as possible prior to this stage by editing the manuscript thoroughly. The editorial office will then prepare the manuscripts for typesetting.

2.6.4 Page Proofs

Page proofs will be sent as pdf files to the author and volume editor for correction. Corrections can be added to the pdf using the commenting tools available within Adobe Acrobat (or other software for handling pdf documents). It is also acceptable for authors to print the proofs, mark up corrections by hand, and send a scan of the proofs to the editorial office by e-mail (science-of-synthesis@thieme.de). If neither of these options is feasible, it is also acceptable to send a list of corrections in a simple email or Word document. In such cases, please make sure it is completely clear where the changes should be made (e.g., “page 2, line 3: change X to Y”).

The correction of page proofs should usually be limited to the correction of existing errors and should not involve major changes/additions to the text. If more extensive corrections are necessary as a result of significant new developments, the volume editor and editorial office should be consulted.

Please note that the symbols ■■■ in the proofs indicate that something was missing or unclear in the manuscript and the pertinent information should be added during correction.

The page proofs should be returned to the editorial office by the deadline given. The author and volume editor then sign the page proofs as a permission to publish the manuscript (Imprimatur). By accepting a manuscript, the publisher acquires all rights, in particular copyright and the right of translation. The proof sheets are not indicative of the quality of the final typesetting.

Please note that the editorial office also carries out an in-house proofread, usually after authors and volume editors have returned their corrections to the proofs. Authors may be contacted by the proofreader to resolve any questions that arise during these checks.

The final page layout of the contribution follows the proof correction, i.e. the text is laid out to the exact page length, the pages are numbered, and tables, schemes, and figures are placed as near as possible to the positions indicated by the author and volume editor in the page proofs.

3 Frequently Asked Questions

Below are some common questions asked by authors during the writing process, along with the relevant answers. If you have any additional questions, please do not hesitate to contact the [editorial office](#) for advice.

Q: Does the document template have to be used?

A: Yes, please do. It is important for manuscript processing that the appropriate style names (e.g., H_Method) are attached to the heading paragraphs for each section. It is not important that formatting properties such as the font size, line spacing, or the number of lines per page match the document template. Please feel free to change these properties as long as the style naming is not affected. However, note that any formatting options in the document processing program except the style names are deleted after manuscript submission. Please note that layout of the manuscripts in the document template does not reflect the layout/appearance of the typeset manuscript.

Q: How should I handle tables?

A: Tables and Schemetables should be composed using the table set-up tools of Word. Tables should be placed in the appropriate position in the body of the text. The tables should be labeled clearly with a caption, e.g. <Table 1> Table Caption^[ref nos]. Please *do not* construct tables in ChemDraw.

Q: What structure drawing program should I be using?

A: If possible, please create schemes and figures using ChemDraw. If you do not have access to ChemDraw, the use of other drawing programs will be accepted, but this may result in longer manuscript processing times as a result of redrawing.

For graphics that show other items/images that chemical structures and reactions, other tools may be used but the submitted graphic files (tif, jpf, etc.) should be in good resolution (at least 300 dpi).

Q: How should I handle graphics in tables?

A: State the file name of the graphic (e.g., Table1_01.cdx) in the required position in the table in the Word document. Save the graphic as a separate ChemDraw file, making sure that the file name corresponds to that given in the table cell.

Q: Is it possible to handle several schemes in one file?

A: No. Each scheme should be saved in a separate file, as should any figures, using the scheme or figure number as the file name e.g. scheme1.cdx.

Q: Can I use colors in graphics?

A: In principle, yes. However, the use of color should be reserved for instances where it provides a clear advantage in terms of the appearance of a scheme or figure. Routine chemical structures and reactions should be in black/white (or greyscale). Note that the use of colour in the abstract graphic is encouraged.

Q: What are the page extent rules for manuscript submission?

A: The volume editors and authors are requested to be aware of the contracted page extent as outlined in the Contributor's Agreement, and to try not exceed the given number of pages for each manuscript. For estimating the final length of a contribution, the following general rules should be used:

1 typeset page = 2 Microsoft Word pages (without graphics pasted in)

1 typeset page = 1½ Microsoft Word pages (with graphics pasted into the Word document)

Q: Do I need to use any particular units or abbreviations?

A: Metric units should be used throughout the text. However, for pressure and temperature, Torr/atm/Pa and °C can be used, respectively. The unit kcal is also accepted. The use of abbreviations is recommended in tables, formulas, schemes, and experimental procedures, but not in titles or text. Please see [here](#) for a full list of abbreviations. Recommended journal abbreviations for use in the references are given [here](#).

Q: How should I submit my manuscript?

A: Please submit the complete manuscript by email as a Word document to both the volume editor and the editorial office (the volume coordinator or science-of-synthesis@thieme.de). Please also remember to send all the graphics files (cdx files) separately (preferably as a zip folder), with the files being named in a logical manner so they can be easily matched to the text. Pasting the ChemDraw files in the document template as ChemDraw-editable items is also acceptable.

Q: I have submitted my manuscript and have received a list of questions from the copyeditor. What should I do?

A: Please simply answer the questions in the spaces provided in the document you received from the copyeditor. Please *do not* send a revised version of the manuscript. However, it may be appropriate to send revised ChemDraw files if significant changes are necessary to schemes.

Q: What do the symbols ■■■ in the page proofs mean?

A: The symbols indicate that something is missing or unclear in the manuscript and the author should add the missing information during correction.

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A: Corrections can be added to the pdf using the commenting tools available within Adobe Acrobat (or other software for handling pdf documents). It is also acceptable for you to print the proofs, mark up corrections by hand, and send a scan of the proofs to the editorial office by e-mail.

If neither of these options is feasible, it is also acceptable to send a list of corrections in a simple email or Word document. In such cases, please make sure it is completely clear where the changes should be made (e.g., “page 2, line 3: change X to Y”).

Q: Do I need to apply for copyright permissions?

A: Copyright permission is generally not required for the reproduction of experimental procedures from standard journals or for the graphical depiction of chemical structures/reactions. Copyright permission may be required where other illustrations (e.g., apparatus setup, graphs, photographs) are reproduced. If you require any further information or advice regarding copyright permissions, please contact Dr. Toby Reeve at the editorial office (toby.reeve@thieme.de). It is recommended to do so before making applications directly for the reuse of content.

Q: What is the difference between a General Procedure and a Typical Procedure?

A: A General Procedure is a generalized version of a widely applicable experimental procedure. A Typical Procedure is a specific example of a widely applicable experimental procedure.

Q: How do I cite my chapter in other publications, such as journals?

The recommended citation formats for your contribution will be communicated by the editorial office upon publication of the article. Inclusion of the DOI is recommended. Some examples are provided below.

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