

Scientific Papers

The chemistry community, like other scientific communities, depends on the communication of scientific results. Scientists communicate in a variety of ways, but much of the communication is through publication in books and journals. In this chapter, the different types of book and journal presentations are described, along with the components of the standard format for reporting original research.

Types of Books

Books for the professional scientific community fall into one of three categories: proceedings volumes, monographs, and handbooks.

Proceedings Volumes

Books based on meetings are called proceedings volumes. These are multiauthored volumes. The chapters in proceedings volumes may be accounts of original research or literature reviews. Generally, the chapters are developed and expanded from presentations given at symposia, but additional chapters may be written especially for the book to make sure that the coverage of the topic is complete. Proceedings volumes should contain at least one chapter that reviews the subject and also provides an overview of the book to unify the chapters into a coherent treatment of the subject. In a longer book that is divided into sections, each section may need a short overview chapter.

Monographs

Monographs are books that examine a single topic in detail. They are written by one author or collaboratively by more than one author. Each chapter treats one subdivision of the broader topic.

Handbooks

Handbooks are large, multiauthored volumes that discuss a field in depth. Generally, the individual submissions are short, about three or four pages. Each submission is written by one or two authors and provides a detailed discussion of a narrow topic within the scope of the book.

Journal Presentations

There are four general types of presentations published in journals: articles, notes, communications, and reviews.

Articles

Articles, also called full papers, are definitive accounts of significant, original studies. They present important new data or provide a fresh approach to an established subject. The organization and length of an article should be determined by the amount of new information to be presented and by space restrictions within the publication.

Notes

Notes are concise accounts of original research of a limited scope. They may also be preliminary reports of special significance. The material reported must be definitive and may not be published again later. Appropriate subjects for notes include improved procedures of wide applicability or interest, accounts of novel observations or of compounds of special interest, and development of new techniques. Notes are subject to the same editorial appraisal as full-length articles.

Communications

Communications, called “letters” or “correspondence” in some publications, are usually preliminary reports of special significance and urgency that are given expedited publication. They are accepted if the editor believes that their rapid publication will be a service to the scientific community. Communications are generally subject to strict length limitations; they must contain specific results to support their conclusions, but they may not contain nonessential experimental details.


The same rigorous standards of acceptance that apply to full-length articles also apply to communications. Like all types of presentations in journals, communications are submitted to review. In many cases, authors are expected to publish complete details (not necessarily in the same journal) after their communications have been published. Acceptance of a communication, however, does not guarantee acceptance of the detailed manuscript.

Reviews

Reviews integrate, correlate, and evaluate results from published literature on a particular subject. They seldom report new experimental findings. Effective review articles have a well-defined theme, are usually critical, and may present novel theoretical interpretations. Ordinarily, reviews do not give experimental details, but in special cases (as when a technique is of central interest), experimental procedures may be included. An important function of reviews is to serve as a guide to the original literature; for this reason, accuracy and completeness of references cited are essential.

Standard Format for Reporting Original Research

The main text of scientific papers presenting original research is generally organized into a standard format: abstract, introduction, experimental details or theoretical basis, results, discussion, and conclusions, although not necessarily in this order. This format has become standard because it is suitable for most reports of original research, it is basically logical, and it is easy to use. The reason it accommodates most reports of original research is that it parallels the scientific method of deductive reasoning: define the problem, create a hypothesis, devise an experiment to test the hypothesis, conduct the experiment, and draw conclusions. Furthermore, this format enables the reader to understand quickly what is being presented and to find specific information easily. This ability is crucial now more than ever because scientists, if not all professionals, must read much more material than in the past.

 **Reminder:** Journal articles and proceedings chapters are usually organized with an abstract, introduction, experimental details or theoretical basis, results, discussion, and conclusions.

Use the standard form for reports of original research whether the report is published in a journal or proceedings volume. Even if the information is more suited to one of the shorter types of presentations, the logic of the standard format applies, although some headings or sections may be omitted or other sections and subsections added. Manuscripts for monographs, handbooks,

literature reviews, or theoretical papers generally do not follow the standard form. Consult author guidelines for information on how to organize these types of presentations or look at previously published work. Regardless of the type of presentation, be sure to present all parts of the paper as concisely as possible.

An extremely important step is to check the specific requirements of the publication targeted and follow them. Some publishers provide templates that help authors produce manuscripts in the requested format. Templates are also useful in making sure that the manuscript is not too long. Most editors require revisions of manuscripts that are not in their requested format. Thus, not following a publication's requirements can delay publication and make more work for authors.

Title

The best time to determine the title is after the text is written, so that the title will reflect the paper's content and emphasis accurately and clearly. The title must be brief and grammatically correct but accurate and complete enough to stand alone. A two- or three-word title may be too vague, but a 14- or 15-word title is unnecessarily long. If the title is too long, consider breaking it into title and subtitle.

The title serves two main purposes: to attract the potential audience and to aid retrieval and indexing. Therefore, include several keywords. The title should provide the maximum information for a computerized title search.

- Choose terms that are as specific as the text permits, e.g., “a vanadium–iron alloy” rather than “a magnetic alloy”. Avoid phrases such as “on the”, “a study of”, “research on”, “report on”, “regarding”, and “use of”. In most cases, omit “the” at the beginning of the title. Avoid nonquantitative, meaningless words such as “rapid” and “new”.
- Spell out all terms in the title, and avoid jargon, symbols, formulas, and abbreviations. Whenever possible, use words rather than expressions containing superscripts, subscripts, or other special notations. Do not cite company names, specific trademarks, or brand names of chemicals, drugs, materials, or instruments.
- Series titles are of little value. Some publications do not permit them at all. If consecutive papers in a series are published simultaneously, a series title may be relevant, but in a long series, paper 42 probably bears so limited a relationship to paper 1 that they do not warrant a common title. In addition, an editor or reviewer seeing the same title repeatedly may reject it on the grounds that it is only one more publication on a general topic that has already been discussed at length.


Byline and Affiliation

Include in the byline all those, and only those, who made substantial contributions to the work, even if the paper was actually written by only one person. Chapter 1 and Appendix 1-1 in this book are more explicit on this topic.

- Many ACS publications specifically request at least one full given name for each author, rather than only initials. Use your first name, initial, and surname (e.g., John R. Smith) or your first initial, second name, and surname (e.g., J. Robert Smith). Whatever byline is used, be consistent. Papers by John R. Smith, Jr., J. Smith, J. R. Smith, Jack Smith, and J. R. Smith, Jr., will not be indexed in the same manner; the bibliographic citations may be listed in five different locations, and ascribing the work to a single author will therefore be difficult if not impossible.
- Do not include professional, religious, or official titles or academic degrees.
- The affiliation is the institution (or institutions) at which the work was conducted. If the author has moved to another institution since the work was done, many publications include a footnote giving the current address. Contact the editor about this.
- If there is more than one author, use an asterisk or superscript (check the specific publication's style) to indicate the author or authors to whom correspondence should be addressed. Clarify all corresponding authors' addresses by accompanying footnotes if they are not apparent from the affiliation line. E-mail addresses may be included in corresponding author footnotes.

Abstract

Most publications require an informative abstract for every paper, even if they do not publish abstracts. For a research paper, briefly state the problem or the purpose of the research, indicate the theoretical or experimental plan used, summarize the principal findings, and point out major conclusions. Include chemical safety information when applicable. Do not supplement or evaluate the conclusions in the abstract. For a review paper, the abstract describes the topic, scope, sources reviewed, and conclusions. Write the abstract last to be sure that it accurately reflects the content of the paper.

 **Reminder:** The abstract allows the reader to determine the nature and scope of the paper and helps technical editors identify key features for indexing and retrieval.

- Although an abstract is not a substitute for the article itself, it must be concise, self-contained, and complete enough to appear separately in abstract publications. Often, authors' abstracts are used with little change in abstract pub-

lications. The optimal length is one paragraph, but it could be as short as two sentences. The length of the abstract depends on the subject matter and the length of the paper. Between 80 and 200 words is usually adequate.

- Do not cite references, tables, figures, or sections of the paper in the abstract. Do not include equations, schemes, or structures that require display on a line separate from the text.
- Use abbreviations and acronyms only when it is necessary to prevent awkward construction or needless repetition. Define abbreviations at first use in the abstract (and again at first use in the text).

Introduction

A good introduction is a clear statement of the problem or project and the reasons for studying it. This information should be contained in the first few sentences. Give a concise and appropriate background discussion of the problem and the significance, scope, and limits of the work. Outline what has been done before by citing truly pertinent literature, but do not include a general survey of semirelevant literature. State how your work differs from or is related to work previously published. Demonstrate the continuity from the previous work to yours. The introduction can be one or two paragraphs long. Often, the heading “Introduction” is not used because it is superfluous; opening paragraphs are usually introductory.

Experimental Details or Theoretical Basis

In research reports, this section can also be called “Experimental Methods”, “Experimental Section”, or “Materials and Methods”. Be sure to check the specific publication for the correct title of this section. For experimental work, give sufficient detail about the materials and methods so that other experienced workers can repeat the work and obtain comparable results. When using a standard method, cite the appropriate literature and give only the details needed.

- Identify the materials used and give information on the degree of and criteria for purity, but do not reference standard laboratory reagents. Give the chemical names of all compounds and the chemical formulas of compounds that are new or uncommon. Use meaningful nomenclature; that is, use standard systematic nomenclature where specificity and complexity require, or use trivial nomenclature where it will adequately and unambiguously define a well-established compound.
- Describe apparatus only if it is not standard or not commercially available. Giving a company name and model number in parentheses is nondistracting and adequate to identify standard equipment.

- Avoid using trademarks and brand names of equipment and reagents. Use generic names; include the trademark in parentheses after the generic name only if the material or product used is somehow different from others. Remember that trademarks often are recognized and available as such only in the country of origin. In ACS publications, *do not use* trademark (™) and registered trademark (®) symbols.
- Describe the procedures used, unless they are established and standard.
- Note and emphasize any hazards, such as explosive or pyrophoric tendencies and toxicity, in a separate paragraph introduced by the heading “Caution:”. Include precautionary handling procedures, special waste disposal procedures, and any other safety considerations in adequate detail so that workers repeating the experiments can take appropriate safety measures. Some ACS journals also indicate hazards as footnotes on their contents pages.

In theoretical reports, this section is called, for example, “Theoretical Basis” or “Theoretical Calculations” instead of “Experimental Details” and includes sufficient mathematical detail to enable other researchers to reproduce derivations and verify numerical results. Include all background data, equations, and formulas necessary to the arguments, but lengthy derivations are best presented as supporting information.

Results

Summarize the data collected and their statistical treatment. Include only relevant data, but give sufficient detail to justify the conclusions. Use equations, figures, and tables only where necessary for clarity and brevity. Extensive but relevant data should be included in supporting information.

Discussion

The purpose of the discussion is to interpret and compare the results. Be objective; point out the features and limitations of the work. Relate your results to current knowledge in the field and to the original purpose in undertaking the project: Was the problem resolved? What has been contributed? Briefly state the logical implications of the results. Suggest further study or applications if warranted.

Present the results and discussion either as two separate sections or as one combined section if it is more logical to do so. Do not repeat information given elsewhere in the manuscript.

Conclusions

The purpose of the conclusions section is to put the interpretation into the context of the original problem. Do not repeat discussion points or include irrelevant material. Conclusions should be based on the evidence presented.

Summary

A summary is unnecessary in most papers. In long papers, a summary of the main points can be helpful, but be sure to stick to the main points. If the summary itself is too long, its purpose is defeated.

Acknowledgments

Generally, the last paragraph of the paper is the place to acknowledge people, organizations, and financing. As simply as possible, thank those persons, other than coauthors, who added substantially to the work, provided advice or technical assistance, or aided materially by providing equipment or supplies. Do not include their titles. If applicable, state grant numbers and sponsors here, as well as auspices under which the work was done, including permission to publish if appropriate.

Follow the publication's guidelines on what to include in the acknowledgments section. Some journals permit financial aid to be mentioned in acknowledgments, but not meeting references. Some journals put financial aid and meeting references together, but not in the acknowledgments section.

References

In many books and journals, references are placed at the end of the article or chapter; in others, they are treated as footnotes. In any case, place the list of references at the end of the manuscript.

In ACS books and most journals, the style and content of references are standard regardless of where they are located. Follow the reference style presented in Chapter 14.

The accuracy of the references is the author's responsibility. Errors in references are one of the most common errors found in scientific publications and are a source of frustration to readers. Increasingly, hypertext links are automatically generated in Web-based publications, but this cannot be done for references containing errors. If citations are copied from another source, check the original reference for accuracy and appropriate content.

 **Reminder:** The accuracy of the references is the author's responsibility.

Special Sections

This discussion on format applies to most manuscripts, but it is not a set of rigid rules and headings. If the paper is well organized, scientifically sound, and appropriate to the publication, adding other sections and subsections may be helpful to readers. For example, an appendix contains material that

is not critical to understanding the text but provides important background information.

Supporting Information

Material that may be essential to the specialized reader but not require elaboration in the paper itself is published as supporting information, usually on the journal's Web page. Examples of supporting information include large tables, extensive figures, lengthy experimental procedures, mathematical derivations, analytical and spectral characterization data, biological test data for a series, molecular modeling coordinates, modeling programs, crystallographic information files, instrument and circuit diagrams, and expanded discussions of peripheral findings.

More journals are encouraging this type of publishing to keep printed papers shorter. For ACS journals, supporting information is available immediately by linking to it from the citing paper on the Web. For example, for the article "Vanadium-Based, Extended Catalytic Lifetime Catechol Dioxygenases: Evidence for a Common Catalyst" by Cindy-Xing Yin and Richard G. Finke in *The Journal of the American Chemical Society* **2005**, *127*, 9003–9013, the supporting information consists of two files, ja051594esi20050517_053152.pdf (453 K) and ja051594erom20050320_064528.cif (24 K).

When including supporting information, place a statement to that effect at the end of the paper, using the format specified in the author instructions for the specific journal. For complete instructions on how to prepare this material for publication, check the author instructions for the publication.

Web-Enhanced Objects

Some publishers, including ACS, have started exploring various Web-based technologies to enhance the way that information in a research article is conveyed. Selected papers in Web editions may contain Web-enhanced objects (WEOs) to supplement a reader's understanding of the research being reported. These types of files include color figures (including three-dimensional, rotatable figures), chemical structures, animations, spectra, video, and sound files. Links to WEOs will appear in the Web edition of the paper. These objects, although not essential to the understanding of the science, should help to augment a reader's understanding of the research being reported. The types of objects suitable for this form of publication should be viewable with commonly available plugins (e.g., Chime) or helper applications (e.g., WebLab Viewer, RasMol), which allow viewing and manipulating these objects within the HTML file itself or in a separate window. For example, a figure in the journal article "Orientation and Phase Transitions of Fat Crystals under Shear" by Gianfranco Mazzanti, Sarah E. Guthrie, Eric B. Sirota, Alejandro G. Marangoni, and Stefan H. J. Idziak, in

Crystal Growth & Design **2003**, *3*, 721–725, is supplemented by a movie WEO (in .mov format) depicting the time sequence of synchrotron X-ray diffraction patterns for the crystallization of cocoa butter in chocolate (see <http://pubs.acs.org/isubscribe/journals/cgdefu/asap/objects/cg034048a/Mazzantivideoaip.mov>).

As with other types of special information, authors should check the author guidelines for the publication for instructions on how to prepare and submit WEOs.