The ACS Style Guide
Contents

Foreword .......................................................................................................................... vii
  Madeleine Jacobs
Preface .............................................................................................................................. ix
Contributors ...................................................................................................................... xiii

Part 1. Scientific Communication

1. Ethics in Scientific Communication ........................................................................ 3
   Gordon G. Hammes
   APPENDIX 1-1: Ethical Guidelines to Publication of Chemical Research .......... 11

2. Scientific Papers ....................................................................................................... 17

3. The Editorial Process ............................................................................................... 27
   APPENDIX 3-1: Proofreaders’ Marks ................................................................... 36

4. Writing Style and Word Usage ................................................................................ 41

5. Electronic Submission of Manuscripts Using Web-Based Systems ................... 59
   Sarah C. Blendermann
   APPENDIX 5-1: Online Submission at Selected Scientific Publishers
                 and Research Grant Agencies ........................................................................... 65
   APPENDIX 5-2: Key Features of Selected Online Submission Systems ............... 68

6. Peer Review ............................................................................................................. 71
   Barbara A. Booth

7. Copyright Basics ..................................................................................................... 77
   Karen S. Buehler, C. Arleen Courtney, and Eric S. Slater
# Part 2. Style Guidelines

8. **Markup Languages and the Datument** ........................................... 87  
   *Peter Murray-Rust and Henry S. Rzepa*

   **APPENDIX 8-1:** The IUPAC International Chemical Identifier, InChI .............. 101  
   *Stephen R. Heller and Alan D. McNaught*

9. **Grammar, Punctuation, and Spelling** ............................................ 105  
   **APPENDIX 9-1:** Recommended Spelling List .................................. 129

10. **Editorial Style** ............................................................................ 135  
    **APPENDIX 10-1:** Computer and Internet Terms ................................. 163  
    **APPENDIX 10-2:** Abbreviations, Acronyms, and Symbols. ................. 169

11. **Numbers, Mathematics, and Units of Measure** ............................... 203  
    **APPENDIX 11-1:** The International System of Units (SI) ................. 228

12. **Names and Numbers for Chemical Compounds** .............................. 233  
    **APPENDIX 12-1:** End-of-Line Hyphenation of Chemical Names .......... 247  
    **APPENDIX 12-2:** Representation of Combinatorial Chemistry .......... 250  
    *Derek Maclean*

    **APPENDIX 12-3:** CAS Registry Numbers .................................. 253

13. **Conventions in Chemistry** .......................................................... 255  
    **APPENDIX 13-1:** Symbols for Commonly Used Physical Quantities .... 277  
    **APPENDIX 13-2:** The Crystallographic Information File. ............... 284  
    *Frank H. Allen*

14. **References** .................................................................................. 287  
    *Janet S. Dodd, Leah Solla, and Paula M. Bérard*

    **APPENDIX 14-1:** CASSI Abbreviations for the 1000+ Most Commonly  
    Cited Journals. ........................................................................ 328  
    **APPENDIX 14-2:** A Sample CASSI Entry .................................. 340

15. **Figures** ...................................................................................... 343  
    *Betsy Kulamer*

16. **Tables** ...................................................................................... 369  
    *Betsy Kulamer*

17. **Chemical Structures** ................................................................. 375  
    *Antony Williams*

18. **Selected Bibliography** .................................................................. 385

Index ..................................................................................................... 389
fell in love with chemistry when I was 13. I fell in love with writing at the age of four when I learned to read. Indeed, my love of writing, and of writing well, was inspired by my love of reading. Perhaps that is true for all writers.

Fortunately for me, I have been able to combine my love of chemistry with my love of reading and writing in a long career as a science communicator and journalist. Most recently, I served for eight and a half years as editor-in-chief of Chemical & Engineering News, the flagship newsmagazine of the American Chemical Society. This gave me ample opportunity to read all of the stories in C&EN every week, not once but twice and sometimes three times; write weekly editorials and occasionally longer stories; and indulge my love of chemistry vicariously, as I read the scientific papers we highlighted in C&EN.

But writing is not as easy as reading. Writing and communicating take a great deal of skill and effort. One of my favorite quotations on the subject of writing comes from the novelist John Irving, who observed in The World According to Garp that a writer never reads for fun. It’s true for me. When I read a sentence that is well crafted or even better, a scientific paper that is full of well-crafted sentences, I am always trying to figure out how the author managed to express a complicated idea with such ease and grace.

The goal of The ACS Style Guide is to help authors and editors achieve that ease and grace in all of their communications. To my mind, there’s no reason why scientific papers should not be as easy to read as a good novel. That’s a tall order, I realize, but if you read through this style guide, you will have all the tools
you need to help you achieve that goal. It’s a wonderful reference book that I keep on my bookshelf and refer to often. I hope you will as well.

MADELEINE JACOBS
Executive Director and Chief Executive Officer
American Chemical Society
Since publication of the second edition of *The ACS Style Guide* in 1997, much has changed in the world of scientific communication—and yet, many things remain the same.

During the past eight years, electronic dissemination of scientific, technical, and medical (STM) information has come to fruition. In chemistry, both the American Chemical Society and the Royal Society of Chemistry have made their scientific journals available on the World Wide Web and have digitized their respective publications back to the 19th century. Commercial publishers, who publish most of the world’s chemical information, have likewise made their publications available on the Web. Publications in other scientific disciplines, engineering, and medicine have also taken this digital pathway. Whereas traditional journals continue to be printed and used, electronic delivery has greatly expanded the availability and reading of STM information far beyond what could have ever been envisioned with paper journals. Most manuscripts are now written with de facto standard word-processing software and adhere to formats developed for electronic creation and processing. Most manuscripts are submitted electronically, principally via the Internet on the Web. Communications among editors, reviewers, and authors are now largely electronic, as is communication between editors and production facilities and printers.

Regardless of the mode of information creation and delivery, the necessity for accurate information communicated in a clear, unambiguous manner, coupled with the ethical behavior of all participants, remains the same. As Janet Dodd wrote in the preface to the second edition, “In the midst of all this change, the comforting thought is that one goal of authors and editors has not changed: to communicate information in the most understandable and expedient fashion in
publications of the highest quality. To accomplish that goal, we need guidelines. This book is intended to guide and answer questions for authors and editors, to save them time, and to ensure clarity and consistency.”

Third Edition

The third edition aims to continue such guidance while broadening the scope of the book to accommodate changes in technology and the homogenization of international scientific publishing. New topics in the third edition include chapters on

- ethics in scientific communication;
- submitting manuscripts via the Web;
- preparing and submitting publisher-ready figures, tables, and chemical structures, including information about various software programs to create artwork;
- formatting manuscript references to electronic resources and information on reference-management software; and
- markup languages, in anticipation of the classification and capture of scientific information in yet-to-be-defined structures.

The chapters on peer review, copyright, the editorial process, and writing style and word choice have been extensively rewritten. Although language certainly evolves with time, there have not been substantial changes in English during the past seven years. The chapters on grammar, punctuation, spelling, and conventions in chemistry remain largely the same as in the second edition. The use of typefaces, superscripts and subscripts, Greek letters, special symbols, numbers, mathematics, units of measure, and names and numbers for chemical compounds are generally unchanged, although some of the existing rules have been clarified. Some new rules and examples have been added to reflect new fields in chemistry, such as combinatorial chemistry and chemical biology. In all chapters, errors have been corrected (and almost certainly new errors inadvertently introduced!), and some changes have been made to reflect changes in practice, particularly as related to electronic issues.

Several features have been added to the third edition to improve the readers’ ease of use:

- The contents are reorganized into two sections. The first section, “Scientific Communication”, contains chapters giving readers information on broad topics such as ethics in scientific communication, writing style and word usage, and submission of manuscripts using a Web-based system. The second section, “Style Guidelines”, contains chapters that give specific rules and examples. For instance, in these chapters readers will find infor-
mation on such topics as grammar, punctuation, and spelling; formatting numbers and specialized chemical conventions; when to use special typefaces; how to format references; and how to create figures, tables, and chemical structures.

• Throughout the book, the arrowlike icon (➤) precedes rules. These rules may refer to grammar, word usage, or punctuation rules. Also, the icon may precede rules for creating publisher-ready artwork, rules about styling chemical terms, or rules about formatting names and chemical compounds. Examples are given under the rule to further illustrate it.

• Attention is drawn to particularly important topics by the use of reminders and boxes. Reminders are bounded by horizontal rules and are identified with a small pencil icon (✎); they contain a brief note on a single topic. Boxes are numbered sequentially within each chapter and contain more extensive information on a specific topic. Reminders and boxes that contain ACS-specific information are identified by a small ACS phoenix icon (Phoenix). We believe that identification of these key issues in this manner will be helpful to readers.

Because of the desire on the part of the publisher to increase the use of the third edition of *The ACS Style Guide*, it is being made available on the World Wide Web. It is expected that periodic updates will be made to the electronic edition, which would not be feasible for the printed version. Additionally, if readers would like to request clarification of rules, they may do so by contacting the publisher at styleguide@acs.org or by addressing correspondence to The ACS Style Guide, Books Department, American Chemical Society, 1155 Sixteenth Street, NW, Washington, DC 20036.

Although *The ACS Style Guide* is written with an emphasis on chemistry and, to some extent, a focus on ACS journals, we believe that it has wide applicability to the sciences, engineering, medicine, and other disciplines. Chemistry is a mature science that cuts across virtually all basic and applied sciences.

Science in its broadest sense has always been an international activity. However, there is an increasing trend toward internationalization of scientific communication. For example, for the past several years, the majority of authors publishing in ACS journals reside outside North America. English has become the lingua franca of science in the same way that French once was the international language of diplomacy and commerce. The venerated *Beilsteins Handbuch der Organischen Chemie* has been published in English for a number of years. The prestigious journal *Angewandte Chemie: International Edition in English* conveys internationalization and the English language merely by its title. The premier publications *Science* and *Nature*, both published in English, have broad international authorship and readership. We believe that *The ACS Style Guide* will be a useful tool for the international scientific community using this common language.
Acknowledgments

The editors would like to thank all the chapter authors and reviewers who contributed to this project. In particular, we would like to thank our colleagues in Columbus who provided assistance with all the style guidelines in the book, namely, Todd Michael Janiszewski, Diane Needham, “Ram” Ramaswami Ravi, Teresa Schleifer, and Joe Yurvati. A special thank you goes to Betsy Kulamer and Paula M. Bérard for their skilled editorial efforts. We certainly could not have completed this project without their capable assistance. We want to thank Sue Nedrow, who prepared an in-depth index that we think will be very useful to the readers. We also wish to express our appreciation to Bob Hauserman at the ACS for his suggestions and help.

Finally, we would like to express our indebtedness to Janet S. Dodd, who edited the first and second editions of *The ACS Style Guide*. Janet was more than the editor; she wrote much of the first two editions. Her contributions persist in the third edition.

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April 2006
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The principles that govern the ethics of scientific publication are no different than for any other endeavor: complete and accurate reporting and appropriate attribution to the contributions of others. However, as always, “the devil is in the details.” The ethical responsibilities of authors and reviewers are sufficiently important and complex that the editors of the American Chemical Society journals have developed a detailed document outlining these responsibilities. (This document, “Ethical Guidelines to Publication of Chemical Research” is presented in Appendix 1-1.) The purpose of this chapter is not to duplicate this document, but rather to discuss some of the important underlying principles and situations that often arise.

Scientific research, perhaps more than most professions, crucially depends on the integrity of the investigators. Most research consists of a series of complex experiments or theoretical calculations that cannot (or will not) be duplicated easily elsewhere. Moreover, it is usually extremely difficult to determine in detail if the results are correct and can be trusted. Published results generally are accepted at face value. Very often related work eventually may be done by others that tests the results, so that checks and balances exist within the system. This is usually a long process, however, and the advance of science may be significantly delayed if published results are not correct. The bottom line is that we depend on the integrity of the investigators reporting the results. We assume that the description of the work is accurate and honest unless proven otherwise. This places a considerable burden on the authors to ensure that the system works.

Research is by its nature exploratory, and honest mistakes may occur. Errors due to human fallibility are unfortunate, but not unethical. Research inevitably
The ACS Style Guide

pushes the boundaries of existing methodology and theory, so that errors in judgment and interpretation are bound to occur. This is a normal part of the scientific establishment. An often-quoted adage is that the only way never to make a mistake in print is never to publish. Errors due to carelessness or haste are poor science; they represent irresponsible, but not unethical, behavior.

Errors due to fabrication and falsification clearly are unethical and cannot be tolerated under any circumstances. Breakdowns in the system that are not honest mistakes have occurred; some examples are published by the Office of Research Integrity of the U.S. Department of Health and Human Services at http://ori.dhhs.gov. Fortunately, these breakdowns seem to be relatively few.

It is the responsibility of each author to ensure the quality and integrity of the research that is reported. The ethical principles governing the conduct of science should be well understood by all participants. This chapter considers only some aspects of this subject. An excellent introductory publication is available online from the National Academy of Sciences; see “On Being a Scientist: Responsible Conduct in Research” at http://www.nap.edu/readingroom/books/obas/.

When To Publish: Significance and Timeliness

When is it time to publish? Research is open-ended, so the answer to this question is not always obvious and requires authors to balance significance and timeliness to arrive at a high-quality manuscript.

Reminder: Research should be published in a timely manner when enough work has been done to yield significant results.

Researchers must decide when enough work has been done to make a significant contribution to a field. “Significant” is in the eye of the beholder, and sometimes reviewers and authors will differ markedly with regard to this judgment. The give and take between authors and reviewers is part of the normal process of science and undoubtedly improves the quality of published work. Clearly neither science nor scientific publishing are enhanced by a continual stream of short, incomplete descriptions of a research project. A publication should describe a project that is complete unto itself and represents a true advance in the field. (An exception to this rule occurs when a very unusual result is obtained that is of great interest and significance—in this case, publication as a preliminary note may be justified.)

Scientists also have an obligation to publish their research results in a timely manner. Unpublished research results constitute research not done in the eyes of other scientists. Unnecessary delays can result in duplication of efforts and may hinder the advancement of science. Under no circumstances should a manuscript
be submitted and then held up in the revision or page proof stage for reasons not
directly related to the research—for example, because of patent considerations.

Given the “publish or perish” mentality that sometimes exists, researchers
may be tempted to maximize their number of publications by publishing many
short, somewhat repetitive research reports. This practice serves no useful pur-
pose for science or the investigator. In truth, the reputation of an investigator is
ultimately determined by the quality of research done over an extended time.
Beginning independent investigators are often told that a research reputation
can be thought of as a product of quantity times quality of published work. If
only one publication appears every 10 years, they may be advised, it had better
be a good one. On the other hand, a large number of low-quality publications is
not of benefit to the individual or the profession.

Investigators may be tempted to publish the same material, or material only
slightly different, multiple times. This practice is unethical. The manuscript should
clearly describe prior work that has been done by the authors. It is the obligation
of the corresponding author to inform the journal editor of any related manu-
scripts that have been submitted and/or published elsewhere, including prelimi-
nary communications and symposium volumes. There are no exceptions. More-
over, although the review process can be lengthy, under no circumstances should a
manuscript be submitted simultaneously to multiple journals.

What To Publish: Full Disclosure

Unfortunately, because of space limitations, the trend in publishing research
results is to provide less and less detail. Although brevity is admirable, it is impor-
tant that the results be described fully and accurately. Moreover, all of the results
should be reported, not just those supporting the underlying hypotheses of the
research. If necessary, most journals allow the possibility of submitting support-
ing documentation as supplementary information. Although this material does
not appear in the printed version, it is readily available online. The rule of thumb
is that sufficient information should be provided so that other investigators could
repeat the experiments if they so desired. The necessity for providing sufficient
detail has to be balanced with the need to conserve publication space. As might
be expected, considerable variation exists in practice as to what this entails. The
manuscript review process plays a tempering role, balancing these two factors.

Representative data and/or calculations are an important part of any scien-
tific presentation. Obviously, not all of the data, derivations, and calculations can
be presented. It is acceptable for the “typical data and/or calculations” that are
presented to be among the best, but all the data should be included in the analy-
ses. The reproducibility of the results is an implicit assumption for published
work. However, first-rate research often involves difficult measurements at the
edge of existing methodology, and the difference between signal and noise may
be hard to distinguish. It is acceptable to report results for which this is the case, as long as the appropriate qualifications are clearly stated. A critical assessment of the research should be made by the investigator, including an error analysis. No one should be more critical of the research that is reported than the authors.

Who Are Authors?

Generally speaking, all authors of a publication should have made significant and substantial intellectual contributions to the work being reported. Unfortunately, this principle is often breached, as evidenced by manuscripts with tens, even hundreds, of authors. Some laboratories put the names of everyone in the laboratory on the published work, and some individuals put their names on every publication coming out of a laboratory, even if their participation was only nominal.

If a colleague prepared buffers or did routine computer programming, these contributions should be acknowledged, but they are not sufficient contributions for authorship. General discussion with colleagues or within research groups is rarely sufficient for inclusion in authorship. Despite some arbitrariness in defining what constitutes a significant intellectual contribution, the guiding ethical principle is clear and should be adhered to. Usually the question of authorship can be decided by discussion among the participants in the research. Occasionally, a third party may be required to adjudicate this issue. In any event, this matter should be fully resolved before submission of a manuscript.

A question that often arises concerns the order of the authors’ names. This is not really an ethical issue, and practice varies from place to place. Most often the first author is assumed to have made the major contribution to the work, and the senior and/or corresponding author is listed last. However, many variations to this theme exist, such as putting the authors in alphabetical order. In some cases, the specific contributions of each author are described. Ideally, the order of authorship should be decided amicably among the authors, but perceptions sometimes differ between the individuals involved. Authors should not become obsessed with this matter. Ultimately, a researcher’s scientific reputation rests on the totality of publications and the significance of contributions to the field.

It is often said that all authors are responsible for the entire content of a manuscript. This is a meritorious ideal, but unrealistic. Most manuscripts have multiple authors, and very often, a single author is responsible for only a portion of the work being presented. For example, the manuscript may contain a crystal structure, determined by an expert crystallographer; spectral data, determined by an expert spectroscopist; kinetic data, determined by an expert kineticist; etc. In cases such as this, a single author cannot be held responsible for all of the results presented. A more realistic assessment of what authorship implies is that each author should have read the manuscript carefully and understood the findings, but the technical responsibility is only for the area in which a given author
has the appropriate expertise. The responsibility of the corresponding author is to ensure that all authors have approved the manuscript before submission and for all subsequent revisions.

**What Went Before: Attribution and Context**

Every scientific publication must include the proper attribution of the contributions of others by appropriate referencing and the placement of results within the context of the research field.

Referencing is a complex subject (see Chapter 14 of this volume). Every reference in the field cannot be cited, or the reference list would become intolerably long. However, important ideas and experiments must be cited. The introduction and discussion sections of a manuscript should be absolutely clear as to what the work of others has contributed to the research being reported. If data are presented that have been previously published, this should be clearly indicated. Direct quotations of more than a few words should be indicated by quotation marks and referenced. Paraphrases of quotations also should be referenced. Plagiarism—taking the writings or ideas of another and passing them off as one’s own—of any type represents unethical conduct.

Occasionally, the attribution of an idea or fact may be to a “private communication” of a colleague or fellow scientist. In such cases, permission must be obtained from the individual in question before the citation is made. Reference to unpublished material should be avoided if possible because it generally will not be available to interested readers.

**Reminder:** Every manuscript must reference the contributions of others and place results in the context of the research field.

The results and conclusions sections of a manuscript should be placed within the context of the research area. What was known before the research being presented? What has this research contributed that is new and significant? It should also be clear what conclusions are based on the work presented and which are speculations. It is appropriate to speculate—in fact, this is a stimulus to the field—as long as speculations are labeled as such. In this regard, the values and judgments of the authors and current thinking appropriately come into play.

Not all attributions to previous work cite supportive data. In some cases, results under discussion may differ from previous work, or authors may make critical comments about earlier research. Differences between the work reported and previous results must be discussed and reconciled. Criticism of previous work should be presented carefully and objectively, in terms of the facts only. This is part of normal scientific discourse. Criticism should never be directed at
individuals or laboratories; it is essential to consider only the facts that have been presented.

Acknowledgments should be made to people who have assisted in the project, but not sufficiently for authorship, and to sponsoring agencies. It is also imperative to acknowledge potential conflicts of interest that may exist. For example, if the research being reported concerns drug XYZ and one of the authors has a substantial financial interest in a company that makes drug XYZ or is conducting clinical trials with drug XYZ, these facts should be explicitly stated.

What Next: After Publication

An author’s obligations do not stop with publication. If errors are found in the published work, they should be corrected with the publication of errata. If other investigators request more information or more complete data, the requests should be fulfilled without delay.

A trickier issue concerns the distribution of special materials used in the research. The rule of thumb is that the authors should be willing to provide others with a reasonable supply of special materials that have been used in the research. However, some common sense should be applied to this rule. For example, if two years have been spent cloning a specific protein and it will be used in future research, it is unreasonable to expect researchers to give this clone to competitors who are planning similar experiments. Similarly, if a complex substance has been synthesized and only a small supply is available, it would be unreasonable to expect the material to be given away. However, the publication should provide sufficient detail so that other researchers can develop the clone themselves or synthesize the compound in question. Although ethical behavior in this area is not always clear, the general rule is that all aspects of the research should be fully disclosed and reasonable assistance should be given to other researchers. Progress in science depends greatly on open communication and cooperation.

Obligations of a Reviewer

Scientific discourse depends on critical review of manuscripts before publication. (Peer review—including ethical considerations—is discussed in greater detail in Chapter 6 of this volume.) The primary obligation of reviewers is to provide a rational, objective review of the science. This requires a careful reading of the manuscript and a careful preparation of the review. The review process is anonymous for most journals, but this does not mean that the reviewer has free rein to criticize. Any criticism must be logically and objectively delineated, and it should never be directed at the authors personally. Reviewers also should place the work within the context of the field: is it a major contribution, minor contri-
bution, or an insufficient contribution to merit publication? Promptness in carrying out reviews is important and an ethical issue. Delaying a publication could be costly to an author, especially in a competitive field. The usual golden rule applies: review with the care and speed you expect for your own manuscripts. If a reviewer cannot meet a deadline, he or she should inform the publisher as soon as possible.

Manuscripts sent to reviewers are confidential documents. Unfortunately, a significant number of reviewers interpret the word “confidential” incorrectly. Confidential does not mean that reviewers can expand the scope of confidentiality, for example, within their research groups, by including a few colleagues, and so on. Confidential documents should not be shared or discussed with anybody without the explicit consent of the journal editor, the editorial board member handling the manuscript, or both. For example, senior investigators sometimes have graduate students or postdoctorals review manuscripts. This is acceptable only if the permission of the editor or editorial board member has been obtained. In some cases, a reviewer may discuss the results with a colleague; this also is forbidden if permission has not been obtained. Although breaches of confidentiality do not usually do any harm and are not intended to do so, they are unethical and should be avoided.

If reviewers have conflicts of interest with regard to a given manuscript, the manuscript should be returned as quickly as possible to the editor. Conflicts of interest vary. Perhaps similar research is being carried out in the reviewer’s laboratory, or the reviewer may be privy to confidential information that conflicts with the results reported. Conflicts of interest can be more personal in nature: perhaps a reviewer has had personal difficulties with or is a close friend of one of the authors. When in doubt, the usual rule is not to review or read the manuscript. If you are unsure, ask the editor handling the manuscript. The editor may want your expert opinion even if some level of apparent conflict exists.

Finally, the results in a manuscript under review cannot be quoted or incorporated into a reviewer’s own research program. After the work is published, a reviewer may use the ideas and data presented (with proper attribution), but the reviewer should not do so based on the review process. Such behavior is akin to insider trading in the purchase of stocks. Although a prison term is unlikely for this breach of conduct, the ethical principle is quite clear.

### Obligations as a Reader

Not all errors are found before publication by authors and reviewers; some are discovered by readers. If the errors involve serious misinterpretation or misquotation of the literature, the most straightforward procedure is to contact the author(s) directly. If this is awkward, the editor can be informed. It is not worthwhile, however, to create a fuss for nonsubstantive errors. Self-serving com-
plaints, such as not quoting the reader’s own work enough, seldom have much credibility.

In rare situations, a scientist may have evidence that published material contains falsification, fabrication, or plagiarism. It is the obligation of every scientist to report such cases immediately to the editor of the journal. Institutions receiving financial support from the National Institutes of Health and the National Science Foundation are required to have mechanisms in place to investigate such occurrences, and direct reporting to the appropriate institutional office may be more expedient. Accusations must be supported by fact, not suspicions, because academic misconduct is a serious matter with career-threatening implications. Unpleasant as this situation may be, it should not be ignored.

**For the Health of Research**

This chapter has emphasized the global ethics of the publication process. Ethics are not complicated, and the practices and rules are mainly common sense. Adherence to ethical standards in research and publication is not optional; rather, it is essential for the health of scientific research.
APPENDIX 1-1

Ethical Guidelines to Publication of Chemical Research

The guidelines embodied in this document were revised by the Editors of the Publications Division of the American Chemical Society in January 2000.

Preface

The American Chemical Society serves the chemistry profession and society at large in many ways, among them by publishing journals which present the results of scientific and engineering research. Every editor of a Society journal has the responsibility to establish and maintain guidelines for selecting and accepting papers submitted to that journal. In the main, these guidelines derive from the Society’s definition of the scope of the journal and from the editor’s perception of standards of quality for scientific work and its presentation.

An essential feature of a profession is the acceptance by its members of a code that outlines desirable behavior and specifies obligations of members to each other and to the public. Such a code derives from a desire to maximize perceived benefits to society and to the profession as a whole and to limit actions that might serve the narrow self-interests of individuals. The advancement of science requires the sharing of knowledge between individuals, even though doing so may sometimes entail forgoing some immediate personal advantage.

With these thoughts in mind, the editors of journals published by the American Chemical Society now present a set of ethical guidelines for persons engaged in the publication of chemical research, specifically, for editors, authors, and manuscript reviewers. These guidelines are offered not in the sense that there is any immediate crisis in ethical behavior, but rather from a conviction that the observance of high ethical standards is so vital to the whole scientific enterprise that a definition of those standards should be brought to the attention of all concerned.

We believe that most of the guidelines now offered are already understood and subscribed to by the majority of experienced research chemists. They may, however, be of substantial help to those who are relatively new to research. Even

The ethical guidelines are also available in their most recent version on the Web at https://paragon.acs.org.
well-established scientists may appreciate an opportunity to review matters so significant to the practice of science.

Guidelines

A. Ethical Obligations of Editors of Scientific Journals

1. An editor should give unbiased consideration to all manuscripts offered for publication, judging each on its merits without regard to race, religion, nationality, sex, seniority, or institutional affiliation of the author(s). An editor may, however, take into account relationships of a manuscript immediately under consideration to others previously or concurrently offered by the same author(s).

2. An editor should consider manuscripts submitted for publication with all reasonable speed.

3. The sole responsibility for acceptance or rejection of a manuscript rests with the editor. Responsible and prudent exercise of this duty normally requires that the editor seek advice from reviewers, chosen for their expertise and good judgment, as to the quality and reliability of manuscripts submitted for publication. However, manuscripts may be rejected without review if considered inappropriate for the journal.

4. The editor and members of the editor’s staff should not disclose any information about a manuscript under consideration to anyone other than those from whom professional advice is sought. (However, an editor who solicits, or otherwise arranges beforehand, the submission of manuscripts may need to disclose to a prospective author the fact that a relevant manuscript by another author has been received or is in preparation.) After a decision has been made about a manuscript, the editor and members of the editor’s staff may disclose or publish manuscript titles and authors’ names of papers that have been accepted for publication, but no more than that unless the author’s permission has been obtained.

5. An editor should respect the intellectual independence of authors.

6. Editorial responsibility and authority for any manuscript authored by an editor and submitted to the editor’s journal should be delegated to some other qualified person, such as another editor of that journal or a member of its Editorial Advisory Board. Editorial consideration of the manuscript in any way or form by the author-editor would constitute a conflict of interest, and is therefore improper.

7. Unpublished information, arguments, or interpretations disclosed in a submitted manuscript should not be used in an editor’s own research except with the consent of the author. However, if such information indicates that some of the editor’s own research is unlikely to be profitable, the editor could
ethically discontinue the work. When a manuscript is so closely related to
the current or past research of an editor as to create a conflict of interest,
the editor should arrange for some other qualified person to take editorial
responsibility for that manuscript. In some cases, it may be appropriate to tell
an author about the editor’s research and plans in that area.

8. If an editor is presented with convincing evidence that the main substance
or conclusions of a report published in an editor’s journal are erroneous, the
editor should facilitate publication of an appropriate report pointing out the
error and, if possible, correcting it. The report may be written by the person
who discovered the error or by an original author.

9. An author may request that the editor not use certain reviewers in consider-
ation of a manuscript. However, the editor may decide to use one or more of
these reviewers, if the editor feels their opinions are important in the fair con-
sideration of a manuscript. This might be the case, for example, when a man-
uscript seriously disagrees with the previous work of a potential reviewer.

B. Ethical Obligations of Authors

1. An author’s central obligation is to present an accurate account of the
research performed as well as an objective discussion of its significance.

2. An author should recognize that journal space is a precious resource created
at considerable cost. An author therefore has an obligation to use it wisely
and economically.

3. A primary research report should contain sufficient detail and reference to
public sources of information to permit the author’s peers to repeat the work.
When requested, the authors should make a reasonable effort to provide sam-
pies of unusual materials unavailable elsewhere, such as clones, microorgan-
ism strains, antibodies, etc., to other researchers, with appropriate material
transfer agreements to restrict the field of use of the materials so as to protect
the legitimate interests of the authors.

4. An author should cite those publications that have been influential in deter-
mining the nature of the reported work and that will guide the reader quickly
to the earlier work that is essential for understanding the present investiga-
tion. Except in a review, citation of work that will not be referred to in the
reported research should be minimized. An author is obligated to perform a
literature search to find, and then cite, the original publications that describe
closely related work. For critical materials used in the work, proper citation
to sources should also be made when these were supplied by a nonauthor.

5. Any unusual hazards inherent in the chemicals, equipment, or procedures
used in an investigation should be clearly identified in a manuscript report-
ing the work.

6. Fragmentation of research reports should be avoided. A scientist who has
done extensive work on a system or group of related systems should organize
publication so that each report gives a well-rounded account of a particular aspect of the general study. Fragmentation consumes journal space excessively and unduly complicates literature searches. The convenience of readers is served if reports on related studies are published in the same journal, or in a small number of journals.

7. In submitting a manuscript for publication, an author should inform the editor of related manuscripts that the author has under editorial consideration or in press. Copies of those manuscripts should be supplied to the editor, and the relationships of such manuscripts to the one submitted should be indicated.

8. It is improper for an author to submit manuscripts describing essentially the same research to more than one journal of primary publication, unless it is a resubmission of a manuscript rejected for or withdrawn from publication. It is generally permissible to submit a manuscript for a full paper expanding on a previously published brief preliminary account (a “communication” or “letter”) of the same work. However, at the time of submission, the editor should be made aware of the earlier communication, and the preliminary communication should be cited in the manuscript.

9. An author should identify the source of all information quoted or offered, except that which is common knowledge. Information obtained privately, as in conversation, correspondence, or discussion with third parties, should not be used or reported in the author’s work without explicit permission from the investigator with whom the information originated. Information obtained in the course of confidential services, such as refereeing manuscripts or grant applications, should be treated similarly.

10. An experimental or theoretical study may sometimes justify criticism, even severe criticism, of the work of another scientist. When appropriate, such criticism may be offered in published papers. However, in no case is personal criticism considered to be appropriate.

11. The coauthors of a paper should be all those persons who have made significant scientific contributions to the work reported and who share responsibility and accountability for the results. Other contributions should be indicated in a footnote or an “Acknowledgments” section. An administrative relationship to the investigation does not of itself qualify a person for coauthorship (but occasionally it may be appropriate to acknowledge major administrative assistance). Deceased persons who meet the criterion for inclusion as coauthors should be so included, with a footnote reporting date of death. No fictitious name should be listed as an author or coauthor. The author who submits a manuscript for publication accepts the responsibility of having included as coauthors all persons appropriate and none inappropriate. The submitting author should have sent each living coauthor a draft copy of the manuscript and have obtained the coauthor’s assent to coauthorship of it.
12. The authors should reveal to the editor any potential conflict of interest, e.g., a consulting or financial interest in a company, that might be affected by publication of the results contained in a manuscript. The authors should ensure that no contractual relations or proprietary considerations exist that would affect the publication of information in a submitted manuscript.

C. Ethical Obligations of Reviewers of Manuscripts

1. Inasmuch as the reviewing of manuscripts is an essential step in the publication process, and therefore in the operation of the scientific method, every scientist has an obligation to do a fair share of reviewing.

2. A chosen reviewer who feels inadequately qualified to judge the research reported in a manuscript should return it promptly to the editor.

3. A reviewer (or referee) of a manuscript should judge objectively the quality of the manuscript, of its experimental and theoretical work, of its interpretations and its exposition, with due regard to the maintenance of high scientific and literary standards. A reviewer should respect the intellectual independence of the authors.

4. A reviewer should be sensitive to the appearance of a conflict of interest when the manuscript under review is closely related to the reviewer’s work in progress or published. If in doubt, the reviewer should return the manuscript promptly without review, advising the editor of the conflict of interest or bias. Alternatively, the reviewer may wish to furnish a signed review stating the reviewer’s interest in the work, with the understanding that it may, at the editor’s discretion, be transmitted to the author.

5. A reviewer should not evaluate a manuscript authored or coauthored by a person with whom the reviewer has a personal or professional connection if the relationship would bias judgment of the manuscript.

6. A reviewer should treat a manuscript sent for review as a confidential document. It should neither be shown to nor discussed with others except, in special cases, to persons from whom specific advice may be sought; in that event, the identities of those consulted should be disclosed to the editor.

7. Reviewers should explain and support their judgments adequately so that editors and authors may understand the basis of their comments. Any statement that an observation, derivation, or argument had been previously reported should be accompanied by the relevant citation. Unsupported assertions by reviewers (or by authors in rebuttal) are of little value and should be avoided.

8. A reviewer should be alert to failure of authors to cite relevant work by other scientists, bearing in mind that complaints that the reviewer’s own research was insufficiently cited may seem self-serving. A reviewer should call to the editor’s attention any substantial similarity between the manuscript under
consideration and any published paper or any manuscript submitted concurrently to another journal.

9. A reviewer should act promptly, submitting a report in a timely manner. Should a reviewer receive a manuscript at a time when circumstances preclude prompt attention to it, the unreviewed manuscript should be returned immediately to the editor. Alternatively, the reviewer might notify the editor of probable delays and propose a revised review date.

10. Reviewers should not use or disclose unpublished information, arguments, or interpretations contained in a manuscript under consideration, except with the consent of the author. If this information indicates that some of the reviewer’s work is unlikely to be profitable, the reviewer, however, could ethically discontinue the work. In some cases, it may be appropriate for the reviewer to write the author, with copy to the editor, about the reviewer’s research and plans in that area.

11. The review of a submitted manuscript may sometimes justify criticism, even severe criticism, from a reviewer. When appropriate, such criticism may be offered in published papers. However, in no case is personal criticism of the author considered to be appropriate.

D. Ethical Obligations of Scientists Publishing outside the Scientific Literature

1. A scientist publishing in the popular literature has the same basic obligation to be accurate in reporting observations and unbiased in interpreting them as when publishing in a scientific journal.

2. Inasmuch as laymen may not understand scientific terminology, the scientist may find it necessary to use common words of lesser precision to increase public comprehension. In view of the importance of scientists’ communicating with the general public, some loss of accuracy in that sense can be condoned. The scientist should, however, strive to keep public writing, remarks, and interviews as accurate as possible consistent with effective communication.

3. A scientist should not proclaim a discovery to the public unless the experimental, statistical, or theoretical support for it is of strength sufficient to warrant publication in the scientific literature. An account of the experimental work and results that support a public pronouncement should be submitted as quickly as possible for publication in a scientific journal. Scientists should, however, be aware that disclosure of research results in the public press or in an electronic database or bulletin board might be considered by a journal editor as equivalent to a preliminary communication in the scientific literature.
he 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 multi-authored 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.
Chapter 2: Scientific Papers

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.

と思いました：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/Mazzantivideouip.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.
CHAPTER 3

The Editorial Process

Publishing a manuscript, whether intended for a journal or a book, is a process. It has four stages: the draft manuscript, manuscript review, the final manuscript, and processing of accepted manuscripts. Along the way, responsibility for the different stages passes from the author, to the journal or book editor, back to the author, and finally to the technical editor. This chapter provides an overview of each of these stages as they evolve in scientific, technical, and medical (STM) publishing.

The Draft Manuscript

Getting Started

Before beginning to write, authors should review the ethical principles of scientific publication (see Chapter 1). The editorial process is supported by the ethical obligations of authors, editors, reviewers, and readers. Author integrity and adherence to the principles that guide scientific publications—such as deciding when it is the appropriate time to publish, determining who should author the manuscript, and providing the proper attribution and context for the research—are as integral to the success of scientific publication as providing science that is sound and of high quality.

Although there is no fixed set of “writing rules” to be followed like a cookbook recipe or an experimental procedure, some guidelines can be helpful. Start by considering the questions in Box 3-1; answering these questions will clarify your goals and make it easier to write the manuscript with the proper amount of detail. It will also make it easier for the book or journal editor to determine the
The ACS Style Guide

manuscript’s suitability for the publication. Writing is like so many other things: once the goal is identified, the details fall into place.

After you have determined the function of the manuscript and identified the audience, review your material for completeness or excess. Reports of original research, whether intended for a journal or a book, can be organized in the standard format: abstract, introduction, experimental details or theoretical basis, results, discussion, and conclusions. These sections are discussed in Chapter 2.

Keep in mind that scientific writing is not literary writing. Scientific writing serves a purpose completely different from that of literary writing, and it must therefore be precise and unambiguous. You and your colleagues probably have been discussing the project for months, so the words seem familiar, common, and clear to you. However, the readers will not have been part of these discussions. Many words are clear when speaking because you can amplify the meaning with gestures, expressions, and vocal inflections—but when these same words are written, they may be clear only to you. Chapter 4 presents strategies on how to write clearly and concisely as well as to select words that convey the meaning intended.

If English is not your first language, ask an English-speaking colleague—if possible, a native English speaker—for help with grammar and diction.

**Publishers’ Requirements**

An extremely important step is to check the specific requirements of the publication and to follow them. Journals often specify a format, the number of pages,
what software packages or file formats are acceptable, how to cite references, and
many other aspects of manuscript preparation. Requirements can vary from
journal to journal even if the same publisher publishes them. Author guidelines
for journals are generally posted on the Web at the journal’s Web site, and they
are also typically published in the first issue of each year. Book publishers also
have author guidelines that need to be followed to expedite publication. Under-
standing the requirements for the manuscript cannot be overemphasized.

Publishing with ACS: The author guidelines for ACS journals can be
seen at http://paragon.acs.org/paragon/index.jsp (see “Author Informa-
tion”). The author guidelines for ACS books can be found at http://pubs.acs.org/books (see “Info for Authors”).

Some publishers provide templates for authors to use when preparing their
manuscripts. Use of a template makes it easier for authors to control margins,
fonts, and paragraph styles, as well as the length of the manuscript. It also facili-
tates peer review by placing tabular and graphical material near the discussion in
the text and providing journal and book editors with a single file to work with.
Templates are generally available for Windows and Macintosh platforms, and
they can be downloaded from a publisher’s or journal’s Web page.

Publishing with ACS: For ACS journals, templates can be accessed at
http://paragon.acs.org/paragon/index.jsp (see “Download Manuscript
Templates”). For ACS proceedings books, templates are available at
http://pubs.acs.org/books/authorinfo.shtml (see “Request instructions
on how to prepare your camera-ready manuscript”).

Artwork

As you write your draft manuscript, consider where structures, schemes, figures,
and tables could be used appropriately to illustrate or support the material. Well-
placed and well-designed artwork communicates information effectively, but too
much artwork can be distracting.

Few scientists have access to graphic arts professionals. Consequently, chemi-
cal professionals need to know how to prepare art for manuscripts. Fortunately,
software packages are available that can be easily mastered to produce good-
looking graphs, charts, schemes, and structures. Chapters 15, 16, and 17 provide
guidelines on when to use artwork and how to create figures, tables, or chemical
structures and schemes that publishers can use effortlessly. These chapters also
describe how to number figures, tables, structures, and schemes.

Sometimes you may wish to use artwork that has been previously published,
whether from your own publications or from those of other authors. To use pre-
viously published artwork, you must get permission from the copyright holder, which is generally the publisher, even if you wrote the manuscript. Because it can take some time to secure reprint permission, it is a good idea to start obtaining permissions as you prepare your draft manuscript. If you wait until your manuscript is accepted for publication to initiate any permissions correspondence, publication of your manuscript may be delayed because publishers generally will not begin working on a manuscript when permissions are missing. Chapter 7 discusses how to get permission to reprint figures that have been previously published. Publishers’ policies, and forms if required, are generally posted on their Web sites.

Publishing with ACS: Authors can reprint artwork previously published in ACS books and journals in other ACS publications without permission, provided that ACS is the original copyright holder. ACS’s copyright policy and procedures can be found at http://pubs.acs.org/copyright_info.html.

Journals vary in their requirements about where tables and figures are placed in the manuscript. Some journals permit tables and figures to be inserted into the text for the draft but require that the tables and figures be submitted separately in the final manuscript. Other journals request that the tables and figures be embedded in the text. Some publishers accept figures prepared in a wide range of software packages, whereas others specify use of certain drawing programs. Check the specific requirements of the publication targeted before submitting the draft manuscript.

Publishing with ACS: Placement of artwork submitted to ACS journals depends on whether the manuscript is submitted through Paragon or the Paragon Plus environment. Be sure to check the author guidelines for the specific journal.

References

References are an important component of every scholarly manuscript. Having complete and accurate references is the author’s responsibility. Errors in references are one of the most common mistakes authors make. Although correct citations have always been important, the increasing number of hypertext links in Web-based publications makes correct citations more important than ever. Given the volume of manuscripts that publishers produce yearly, technical editors cannot verify each reference in each manuscript.

The citation of references in text is a subject that varies widely from journal to journal and publisher to publisher. There are three ways to cite references in text in ACS publications: superscript numbers, italic numbers in parentheses, or author name and year of publication. Authors are encouraged to check the
author guidelines for a specific publication to find information on citing references. Chapter 14 explains how to cite references in ACS publications and how to format references from a variety of publications, in both print and electronic formats.

**Reminder:** Although correct citations have always been important, the increasing number of hypertext links in Web-based publications makes correct citations more important than ever.

**Revising the Draft Manuscript**

Once you have written your initial draft, the next step is a careful revision with an eye to organization, content, and editorial style, beginning with the questions in Box 3-2. Several chapters in this book are designed to help you communicate clearly. Chapter 9 reviews grammar, punctuation, and spelling. Chapter 10 provides guidelines on stylistic and editorial conventions, such as hyphenation and capitalization. Chapter 10 also includes a large appendix with abbreviations, acronyms, and symbols. Guidelines for using numbers, mathematics, and units of measure are given in Chapter 11. Two other chapters focus on more specific issues related to chemistry. Chapter 12 examines the use of proper chemical nomenclature. It provides rules for general chemistry nomenclature, as well as nomenclature in several specialized areas, such as polymer chemistry, biological chemistry, and combinatorial chemistry. Chapter 13 presents a quick reference guide for the use of typefaces, Greek letters, superscripts and subscripts, and special symbols that are commonly used in chemistry. Chapter 13 also includes an appendix containing symbols for commonly used physical quantities.

**Manuscript Review**

When your draft manuscript is complete, check the journal or book author guidelines again for information on how and where to submit your draft. Some editors request that authors suggest possible reviewers. Some journals require that multiple copies of a draft manuscript be submitted and only accept manuscripts through the mail. Other journals request that the manuscript be submitted electronically via e-mail. Still others, like ACS, are using a Web-based system where authors submit a word-processing file or a PDF. For more information on submitting manuscripts using a Web-based system, see Chapter 5.

Once the editor has reviewed the manuscript and determined that it is appropriate for the publication, the peer-review process begins. Chapter 6 describes peer review and the responsibilities of reviewers and authors.
Box 3-2. Questions for Revising Your Manuscript

Does your manuscript as it is written perform the function—new research, literature review, or topic overview—that you identified before you began your draft? Do you still think the format you selected—journal article, book, book chapter—is the best choice?

Have you explained terms, concepts, and procedures in a way that is appropriate to the audience you identified at the start?

Is your material presented in a logical fashion, so that a reader can easily follow your reasoning?

Is the manuscript too long? If so, what sections could be eliminated or possibly used as supporting information?

Do some sections need to be expanded to further clarify the material?

Are the sentences clear and unambiguous?

Are all the words spelled correctly and technical terms used appropriately?

Did you follow generally accepted conventions—such as those in this book—for communicating math and chemistry?

Could you use another opinion? You may find it helpful to ask a colleague, preferably one who is not closely involved with the research on which the manuscript is based, and preferably a native English speaker, to read and comment on your draft.

The Final Manuscript

If your manuscript is accepted, the editor of the book or journal will return the peer-reviewed manuscript with a cover letter synthesizing the reviewers’ comments and indicating what changes must be made for the final manuscript to be accepted. You, the author, then revise the manuscript accordingly. When you submit your final manuscript, include a cover letter indicating what changes you made. If you decide not to make some of the requested changes, you should write a rebuttal and send it with your final manuscript. For more information, see Chapter 6.

Authors are encouraged to submit all the paperwork with the final, revised manuscript. This includes all necessary permissions correspondence and, if required, a signed form transferring copyright from the author to the publisher. Chapter 7 gives a general introduction to copyright. If the manuscript is transmitted electronically, mail the forms separately.
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Finally, keep a copy of the revised manuscript and all permissions correspondence. You will need the revised manuscript to check against the proofs that your publisher sends. Copies of the permissions correspondence can save you time and effort if the permissions correspondence gets lost or separated from your manuscript.

Processing of Accepted Manuscripts

Journal editors and multiauthored book editors send accepted manuscripts directly to the publisher. Authors of monographs interact directly with the publisher, generally through an acquisitions editor. Accepted manuscripts go through three phases before publication: technical editing, proofing and review by the author, and correction by the publisher.

Technical Editing

During the process of creating a book or journal issue, authors’ electronic word-processing files are manipulated in a variety of ways. Files are tagged to identify data elements for print production and links for online products. Artwork is prepared for both publication media. The manuscript is copyedited to ensure consistency, clarity, and grammatical accuracy; changes are introduced to ensure the use of standard chemical conventions, graphics presentation, and tabular format. Copy editors often contact authors or query them at the proof stage for clarification of material.

Author’s Proof

One author, generally the author to whom correspondence should be addressed, receives a proof of the manuscript for final approval before publication. Papers are not generally released for printing until the author’s proof or other approval has been received. Hence, proofs should be checked and returned promptly according to individual journal or book instructions.

Publishing with ACS: ACS journals request that proofs be returned within 48 hours of receipt.

Authors should check proofs very carefully and submit all of the corrections at one time; see Box 3-3 and Appendix 3-1 for information about reviewing
proofs. Only corrections and necessary changes can be made to proofs. Although all authors may look at the proofs, only the corresponding author should submit corrections. Extensive changes may require editorial approval, which delays publication. Printer’s errors are corrected at no cost to authors, but some publishers charge authors the cost of extensive production work made necessary by their own alterations.

**Publication**

After you return your corrected proofs, the technical editor will review them and ensure that the corrections are made properly.

**ASAP (As Soon As Publishable) Articles**

Many STM publishers, including ACS, publish journal articles on the Web before publishing them in print. Papers accepted for publication in ACS journals will be posted on the “Articles ASAP” page on the journal Web site as soon as they are ready for publication; that is, when the proofs are corrected and all author concerns are resolved. Publication on the Web usually occurs within four working days of receipt of proof corrections; this can be any time from three to six weeks before the date of the printed issue. Once a paper appears on the Web, ACS and the scientific community consider it published.

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**Box 3-3. Tips for Checking Proofs**

- If you are instructed to return changes via the Web, list all corrections, revisions, and additions and clearly identify their location.
- If you are instructed to return changes in hard copy (paper printouts), mark corrections legibly in the margins of the proofs as instructed by the publisher. Do not erase or obliterate type; instead, strike one line through copy to be deleted and write the change in the margin.
- Clarify complicated corrections by rewriting the entire phrase or sentence.
- Check all text, data, and references against the original manuscript. Pay particular attention to equations; formulas; tables; captions; spelling of proper names; and numbering of equations, illustrations, tables and references.
- Answer explicitly all queries made by the technical editor.

Proofreader’s marks and a sample of marked manuscript are given in Appendix 3-1.
Article Reprints and Complimentary Copies
Generally, authors receive a form for reprint orders with the author proof. Authors should follow the instructions on the form. Some publishers provide electronic reprints, as well as paper reprints. Customarily, there is a charge for paper reprints, and reprints with color artwork cost more.

Book authors sometimes also receive complimentary copies of the volume in which their chapter appears. On contributions with more than one author, the number of complimentary copies is generally limited; that is, not all authors will receive complimentary copies.

Corrections to Published Manuscripts
Corrections of consequence to a paper that has already been published should be sent to the editor. Most journals publish corrections soon after they have been received. Some journals have a specific format for additions or corrections; check the author guidelines. In books, errata sheets will be printed and included in every book, and the book itself will be corrected before reprinting. However, additions and corrections generally reflect poorly on the authors, and careful manuscript preparation and attention to detail in the entire publication process can prevent the necessity for subsequent corrections.
APPENDIX 3-1

Proofreaders’ Marks

Publishers long ago established conventions for marking changes to manuscripts and proofs. These conventions, known as *proofreaders’ marks*, evolved as an economical and precise shorthand for indicating on paper various types of changes.

Changes to double-spaced manuscript are marked one way (Figure 3A-1). Authors may be called on to interpret these proofreaders’ marks if the publisher has copyediting done by hand, on paper. Common proofreaders’ marks for manuscripts are presented in Figure 3A-2. Note that corrections to manuscripts are made in place (not in the margins) and usually need no additional explanation.

Changes to typeset proofs are marked somewhat differently (Figure 3A-3). Authors may be called on to use this proofreading method if the publisher supplies hard-copy (paper) proofs. Common proofreaders’ marks for proofs (also called *galleys* or *page proofs*) are presented in Figure 3A-4. Note that corrections to proofs are made in two places: a minimal mark is made in the typeset text, to indicate where a change is being made, and an explanatory mark is made in the margin to describe the exact change. For example, a carat mark (^) in the typeset text indicates where new words are to be inserted; the words themselves are written in the margin. If there is more than one change to a typeset line, the changes in the margin are separated by slashes. (If you want to insert a slash, you should write out the word “slash” and circle it in the margin.) Two slashes in a row indicate that the first correction should be repeated. Try not to black out or obliterate the typeset characters. Avoid using arrows and lines to indicate where corrections go because more than one or two on a page breed confusion.
The photochemistry of $\alpha, \beta$-unsaturated ketones has attracted much attention and is still a field of current interest. Numerous examples of such photochemical transformations are well-documented for cyclic enones and dienones, including both cycloaddition reactions and rearrangements. For example, cyclopentenones 1 and 2 readily rearrange to cyclopropyl ketenes upon irradiation. Recently, the related cyclohexadienone-butadienyl ketene rearrangement has been shown to be a highly useful tool in the synthesis of natural products and macrocyclic lactones.

Whereas cis,trans isomerization, photodimerization, and [2 + 2] cycloadditions of acyclic $\alpha, \beta$-unsaturated ketones are well-investigated photochemical transformations, comparatively little is documented concerning the photochemistry of such enones involving photodissociation, rearrangement, or both. Clearly, the absence of ring strain lowers the reactivity toward bond cleavage and renders an initial Norrish type I reaction unlikely. Introduction of radical stabilizing groups in the $\alpha$-position of the enone may, however, be expected to change the reactivity of the enone in favor of the photochemical $\alpha$-cleavage and subsequent reactions derived from the resulting radical pairs.

Figure 3A-1. Sample of a manuscript copyedited by hand.
The photochemistry of α,β-unsaturated ketones has attracted much attention and is still a field of current interest. Numerous examples of such photochemical transformations are well-documented for cyclic enones and dienones, including both cycloaddition reactions and rearrangements. For example, cyclopetenones χ and 2 readily rearrange to cyclopropyl ketenes upon irradiation. Recently, the related cyclohexadienone/butadienyl ketene rearrangement has been shown to be a highly useful tool in the synthesis of natural products and macrocyclic lactones.

Whereas cisfrantsomerization, photodimerization, and [2 + 2] cycloadditions of acyclic α,β-unsaturated ketones are well-investigated photochemical transformations, comparatively little is documented concerning the photochemistry of such enones involving photodissociation, rearrangement or both. Clearly, the absence of ring strain lowers the reactivity toward bond cleavage and renders an initial Norrish type I reaction unlikely. Introduction of radical stabilizing groups in the α-position of the enone may, however, be expected to change the reactivity of the enone in favor of the photochemical α-cleavage and subsequent reactions derived from the resulting radical pairs.

Figure 3A-3. Sample of a marked proof.
Chapter 3: The Editorial Process  ➤  39

Operational Signs
Delete
Close up; delete space
Delete and close up
Insert space
Begin new paragraph
Run paragraphs together
One em space
Move right
Move left
Center
Move up
Move down
Align horizontally
Align vertically
Transpose
Spell out
Let it stand
Flush left
Flush right
Center

Typographical Signs
Lowercase a capital letter
Capitalize a lowercase letter
Set in small capitals
Set in italic type
Set in roman type
Set in boldface type
Wrong font; set in correct type
Superscript
Subscript
Punctuation Marks
Insert comma
Insert apostrophe (or single quotation mark)
Insert quotation marks
Insert period
Insert question mark
Insert semicolon
Insert colon
Insert hyphen
Insert em dash
Insert en dash

Figure 3A-4. Common proofreaders’ marks for marking proofs.
CHAPTER 4

Writing Style and Word Usage

Every writer has a personal style, but all good writing tends to observe guidelines and conventions that communicate meaning clearly and exactly to readers. Scientific writing, in particular, must be precise and unambiguous to be effective.

This chapter presents guidelines for correct sentence structure and word usage. Other chapters of this book present topics also related to good writing style. Chapter 2 discusses the parts of a scientific paper; Chapter 3 presents an overview of the editorial process. Chapters in Part 2 address more specialized rules for usage; see, especially, Chapter 9 on grammar, punctuation, and spelling and Chapter 10 on editorial style.

Correct Sentence Structure

Good organization (see Chapter 2) and sentence structure are an author’s primary tools for conveying information in a logical, persuasive manner. When the words in a sentence are placed so that the reader follows easily from one fact or point to the next, then the reader is best able to comprehend the author’s intended meaning. Poorly structured or ordered sentences create confusion for readers, who are then unable to understand accurately the author’s meaning.

Short, simple declarative sentences—that is, sentences that make statements, rather than pose questions, issue commands, or exclaim—are the easiest to write and the easiest to read. They are also usually clear. However, too many short sentences in a row can sound abrupt or monotonous. They also can place too heavy a burden on the reader to connect the ideas from one sentence to the next. To
add sentence variety and to enhance the flow of ideas, it is better to start with simple declarative sentences and then combine some of them, rather than to start with long rambling sentences and then try to shorten them. Two or more *simple* sentences (sentences with one independent clause and no subordinate clauses) can be combined to form a *compound* sentence. A *complex* sentence is created by adding one or more subordinate clauses to a simple sentence. A *clause* is a group of words that has a subject and a verb. If a clause can stand all by itself, it is an *independent clause*. If a clause cannot stand alone, it is a *dependent* or *subordinate* clause.

**Verbs**

**Voice**

A sentence is said to be in *active voice* when the subject of the sentence is the doer of the action indicated by the verb. The subject of an active verb is doing the action of the verb. In *passive voice*, the subject is the receiver of the action indicated by the verb.

➤ Use the active voice when it is less wordy and more direct than the passive.

**Poor**

The fact that such processes are under strict stereoelectronic control is demonstrated by our work in this area.

**Better**

Our work in this area demonstrates that such processes are under strict stereoelectronic control.

➤ Use the passive voice when the doer of the action is unknown or not important or when you would prefer not to specify the doer of the action.

The solution is shaken until the precipitate forms.
Melting points and boiling points have been approximated.
Identity specifications and tests are not included in the monographs for reagent chemicals.

**Tense**

Using the appropriate verb tense helps to orient the reader as to the nature of the information.

➤ Simple past tense is correct for stating what was done, either by others or by you.

The solutions were heated to boiling.
Jones reviewed the literature and gathered much of this information. We found that relativistic effects enhance the bond strength. The structures were determined by neutron diffraction methods.

➤ Present tense is correct for statements of fact.

Absolute rate constants for a wide variety of reactions are available. Hyperbranched compounds are macromolecular compounds that contain a branching point in each structural repeat unit.

➤ Present and simple past tenses may both be correct for results, discussion, and conclusions.

The characteristics of the voltammetric wave indicate that electron transfer occurs spontaneously. The absence of substitution was confirmed by preparative-scale electrolysis. IR spectroscopy shows that nitrates are adsorbed and are not removed by washing with distilled water.

However, the use of present or simple past tense for results, discussion, and conclusions should be consistent within a paper.

Other Forms

➤ It is acceptable to use split infinitives to avoid awkwardness or ambiguity.

**AWKWARD**

The program is designed to assist financially the student who is considering a career in chemistry.

**BETTER**

The program is designed to financially assist the student who is considering a career in chemistry.

**AMBIGUOUS**

The bonded phases allowed us to investigate fully permanent gases.

**BETTER**

The bonded phases allowed us to fully investigate permanent gases.

**Subjects and Subject–Verb Agreement**

➤ Use first person when it helps to keep your meaning clear and to express a purpose or a decision.

Jones reported xyz, but I (or we) found ....
I (or we) present here a detailed study ....
My (or our) recent work demonstrated ....
To determine the effects of structure on photophysics, I (or we) ....

However, avoid clauses such as “we believe”, “we feel”, and “we can see”, as well as personal opinions.

Subjects and verbs must agree in person and number; this important point is discussed in detail in Chapter 9.

**Sentence Modifiers**

Modifiers made up of phrases or dependent clauses can be added to simple sentences to indicate, for example, cause and effect, or time sequence, or comparison.

- A *restrictive* phrase or clause is one that is essential to the meaning of the sentence. Restrictive modifiers are not set off by commas.
  
  Only doctoral students who have completed their coursework may apply for this grant.
  
  Several systems that take advantage of this catalysis can be used to create new palladium compounds.

- A *nonrestrictive* phrase or clause is one that adds meaning to the sentence but is not essential; in other words, the meaning of the basic sentence would be the same without it. Nonrestrictive modifiers are set off by commas.
  
  Doctoral students, who often have completed their coursework, apply for this teaching fellowship.
  
  Several systems, which will be discussed below, take advantage of this catalytic reaction.

- A *misplaced modifier* is one that is placed next to the wrong word in the sentence, so it inadvertently misrepresents the author’s intended meaning.

  **INCORRECT**
  
  We commenced a new round of experiments unable to point to meaningful conclusions.
  
  **CORRECT**
  
  Unable to point to meaningful conclusions, we commenced a new round of experiments.
➤ A *dangling modifier* is one that lacks a word in the sentence to modify in a logical or sensible way. It should not be confused with an *absolute construction*, which modifies an entire sentence. (See also the discussion of dangling modifiers in Chapter 9.)

**Incorrect**

Adding 2 mL of indicator solution, the end point for the titration was reached.

**Correct**

Adding 2 mL of indicator solution, we reached the end point for the titration.

When we added 2 mL of indicator solution, the end point for the titration was reached.

**Sentence Construction and Word Order**

➤ Use an affirmative sentence rather than a double negative.

<table>
<thead>
<tr>
<th>Instead of</th>
<th>Consider Using</th>
</tr>
</thead>
<tbody>
<tr>
<td>This reaction is not uncommon.</td>
<td>This reaction is common.</td>
</tr>
<tr>
<td>This reaction is not rare.</td>
<td>This reaction is not rare.</td>
</tr>
<tr>
<td>This reaction occurs about 40% of the time.</td>
<td>This reaction occurs about 40% of the time.</td>
</tr>
</tbody>
</table>

This transition was not unexpected. This transition was expected.

We knew that such transitions were possible.

This strategy is not infrequently used. This strategy is frequently used.

This strategy is occasionally used.

This result is not unlikely to occur. This result is likely to occur.

This result is possible.

➤ Watch the placement of the word “only”. It has different meanings in different places in the sentence.

Only the largest group was injected with the test compound. (Meaning: and no other group)

The largest group was only injected with the test compound. (Meaning: and not given the compound in any other way)

The largest group was injected with only the test compound. (Meaning: and no other compounds)

The largest group was injected with the only test compound. (Meaning: there were no other test compounds)

➤ Be sure that the antecedents of pronouns are clear; in other words, when you use a pronoun (for example, “he”, “she”, “it”, or “they”), the noun to which the pronoun refers should be obvious (for example, “Isaac Newton”, “Marie Curie”,...
“the compound”, or “the research team”). This is particularly true for the pro-
nouns “this” and “that”. If there is a chance of ambiguity, use a noun to clarify
your meaning.

**AMBIGUOUS**

The photochemistry of transition-metal carbonyl complexes has been the focus
of many investigations. This is due to the central role that metal carbonyl com-
plexes play in various reactions.

**UNAMBIGUOUS**

The photochemistry of transition-metal carbonyl complexes has been the focus
of many investigations. This interest is due to the central role that metal carbonyl
complexes play in various reactions.

➤ Use the proper subordinating conjunctions. (*Conjunctions join parts of a sen-
tence; subordinating conjunctions join subordinate clauses to the main sentence.*)

“While” and “since” have strong connotations of time. Do not use them where
you mean “although”, “because”, or “whereas”.

**POOR**

Since solvent reorganization is a potential contributor, the selection of data is
very important.

**BETTER**

Because solvent reorganization is a potential contributor, the selection of data is
very important.

**POOR**

While the reactions of the anion were solvent-dependent, the corresponding
reactions of the substituted derivatives were not.

**BETTER**

Although the reactions of the anion were solvent-dependent, the corresponding
reactions of the substituted derivatives were not.

The reactions of the anion were solvent-dependent, but (or whereas) the corre-
sp nding reactions of the substituted derivatives were not.

**Parallelism**

Parallelism, or parallel construction, is the use of words or groups of words of
equal grammatical rank. *Equal grammatical rank* means that words are con-
nected only to words, phrases only to phrases, subordinate clauses only to other
subordinate clauses, and sentences only to other sentences. Establish parallel
construction by using coordinating conjunctions, correlative conjunctions, and
correlative constructions.
A *coordinating conjunction* is a single word, such as “and”, “but”, “or”, “nor”, “yet”, “for”, and sometimes “so”.

**INCORRECT**

Compound 12 was prepared analogously and by Lee’s method (5).

**CORRECT**

Compound 12 was prepared in an analogous manner and by Lee’s method (5).

A *correlative conjunction* is a pairing of words, such as “either … or”; “neither … nor”; “both … and”; “not only … but also”; and “not … but”.

**INCORRECT**

The product was washed either with alcohol or acetone.

**CORRECT**

The product was washed with either alcohol or acetone.

The product was washed either with alcohol or with acetone.

**INCORRECT**

It is best to use alternative methods both because of the condensation reaction and because the amount of water in the solvent increases with time.

**CORRECT**

It is best to use alternative methods both because of the condensation reaction and because of the increase in the amount of water in the solvent with time.

**INCORRECT**

Not only was the NiH functionality active toward the C-donor derivatives but also toward the N donors.

**CORRECT**

The NiH functionality was active not only toward the C-donor derivatives but also toward the N donors.

The NiH functionality was not only active toward the C-donor derivatives but also active toward the N donors.

Not only was the NiH functionality active toward the C-donor derivatives, but it was also active toward the N donors.

**INCORRECT**

Not only was the NiH functionality active toward the C-donor derivatives but also toward the N donors.

**CORRECT**

The NiH functionality was active not only toward the C-donor derivatives but also toward the N donors.

The NiH functionality was not only active toward the C-donor derivatives but also active toward the N donors.

Not only was the NiH functionality active toward the C-donor derivatives, but it was also active toward the N donors.

A *correlative construction* is a sentence structure that uses “as … as” (for example, “as well as”).

He performed the experiment as well as I could have done it.
Do not try to use parallel construction around the word “but” when it is not used as a coordinating conjunction.

Increasing the number of fluorine atoms on the adjacent boron atom decreases the chemical shift, but only by a small amount.

The reaction proceeded readily, but with some decomposition of the product.

Use parallel constructions in series and lists, including section headings and subheadings in text and tables and listings in figure captions.

**Comparisons**

Introductory phrases that imply comparisons should refer to the subject of the sentence and be followed by a comma.

**INCORRECT**

Unlike alkali-metal or alkaline-earth-metal cations, hydrolysis of trivalent lanthanides proceeds significantly at this pH.

**CORRECT**

Unlike that of alkali-metal or alkaline-earth-metal cations, hydrolysis of trivalent lanthanides proceeds significantly at this pH.

Unlike alkali-metal or alkaline-earth-metal cations, trivalent lanthanides hydrolyze significantly at this pH.

**INCORRECT**

In contrast to the bromide anion, there is strong distortion of the free fluoride anion on the vibrational spectroscopy time scale.

**CORRECT**

In contrast to the bromide anion, the free fluoride anion is strongly distorted on the vibrational spectroscopy time scale.

Use the verb “compare” followed by the preposition “to” when similarities are being noted. Use “compare” followed by the preposition “with” when differences are being noted. Only things of the same class should be compared.

Compared to compound 3, compound 4 shows an NMR spectrum with corresponding peaks.

Compared with compound 3, compound 4 shows a more complex NMR spectrum.

Do not omit words needed to complete comparisons, and do not use confusing word order. The subordinating conjunction “than” is often used to introduce the second element in a comparison, following an adjective or adverb in the comparative degree.
INCORRECT

The alkyne stretching bands for the complexes are all lower than the uncoordinated alkyne ligands.

CORRECT

The alkyne stretching bands for the complexes are all lower than those for the uncoordinated alkyne ligands.

The alkyne stretching bands are all lower for the complexes than for the uncoordinated alkyne ligands.

INCORRECT

The decrease in isomer shift for compound 1 is greater in a given pressure increment than for compound 2.

CORRECT

The decrease in isomer shift for compound 1 is greater in a given pressure increment than that for compound 2.

The decrease in isomer shift in a given pressure increment is greater for compound 1 than for compound 2.

Idioms often used in comparisons are “different from”, “similar to”, “identical to”, and “identical with”. Generally these idioms should not be split.

INCORRECT

The complex shows a significantly different NMR resonance from that of compound 1.

CORRECT

The complex shows an NMR resonance significantly different from that of compound 1.

INCORRECT

Compound 5 does not catalyze hydrogenation under similar conditions to compound 6.

CORRECT

Compound 5 does not catalyze hydrogenation under conditions similar to those for compound 6.

EXCEPTION These idioms can be split if an intervening prepositional phrase modifies the first word in the idiom.

The single crystals are all similar in structure to the crystals of compound 7.

Solution A is identical in appearance with solution B.
Phrases such as “relative to”, “as compared to”, and “as compared with” and words such as “versus” are also used to introduce the second element in a comparison. The things being compared must be parallel.

The greater acidity of nitric acid relative to nitrous acid is due to the initial-state charge distribution in the molecules.

The lowering of the vibronic coupling constants for Ni as compared with Cu is due to configuration interaction.

This behavior is analogous to the reduced Wittig-like reactivity in thiolate versus phenoxide complexes.

Correct Word Usage

The words chosen by a writer are one of the defining characteristics of that author’s style; however, word choice is not governed by style alone. The audience for a paper (as discussed in Chapter 3) must influence a writer’s choice of words so that the writer can select words that are likely to be known to the audience and define the words that are not. The type of document also may influence a writer’s word choices because some documents, such as scientific papers, journal articles, and books, tend to more formal word usage, whereas other documents, such as e-mails, allow less formality.

The choice of the correct word to express meaning begins with a good dictionary, but it also extends to understanding small differences in meaning between two words or phrases that are almost synonymous or that are spelled similarly but have significant differences in meaning. It is best to use words in their primary meanings and to avoid using a word to express a thought if such usage is uncommon, informal, or primarily literary. Many words are clear when you are speaking because you can amplify your meaning with gestures, expressions, and vocal inflections—but when these same words are written, they may be clear only to you.

This chapter presents only a few words and phrases that are commonly misused in scientific writing; consult a good reference on word usage for more comprehensive assistance. (Several such references are listed under the heading “References on Scientific Communication” in Chapter 18.)

Grouping and Comparison Words

Use “respectively” to relate two or more sequences in the same sentence.

The excitation and emission were measured at 360 and 440 nm, respectively. (That is, the excitation was measured at 360 nm, and the emission was measured at 440 nm.)
➤ Use the more accurate terms “greater than” or “more than” rather than the imprecise “over” or “in excess of”.

greater than 50% (not in excess of 50%)
more than 100 samples (not over 100 samples)
more than 25 mg (not in excess of 25 mg, not over 25 mg)

➤ Use “fewer” to refer to number; use “less” to refer to quantity.

fewer than 50 animals
fewer than 100 samples
less product
less time
less work

➤ However, use “less” with number and unit of measure combinations because they are regarded as singular.

less than 5 mg
less than 3 days

➤ Use “between” with two named objects; use “among” with three or more named or implied objects.

Communication between scientists and the public is essential.
Communication among scientists, educators, and the public is essential.
Communication among scientists is essential.

**Commonly Confused Words and Phrases**

➤ Choose “myself” and “me” depending on your meaning. “Myself” is a reflexive pronoun that is used only in sentences in which “I” is the subject, whereas “me” is used as a direct or indirect object or the object of a preposition. “Myself” is never a substitute for “me”.

Please give a copy of the agenda to Anne and me. (not to Anne and myself)
I myself checked the agenda.
Cheryl and I checked the agenda. (not Cheryl and myself)
The agenda was checked by Barbara and me. (not by Barbara and myself)

➤ Choose “due to”, which means “attributable to”, only to modify a noun or pronoun directly preceding it in the sentence or following a form of the verb “to be”.

Cutbacks due to decreased funding have left us without basic reference books.
The accuracy of the prediction is due to a superior computer program.
Choose “based on” and “on the basis of” depending on your meaning. Phrases starting with “based on” must modify a noun or pronoun that usually immediately precedes or follows the phrase. Use phrases starting with “on the basis of” to modify a verb.

The doctors’ new methods in brain surgery were based on Ben Carson’s work.

On the basis of the molecular orbital calculations, we propose a mechanism that can account for all the major features of alkali and alkaline earth catalyzed gasification reactions. (not Based on …)

Choose “assure”, “ensure”, and “insure” depending on your meaning. To assure is to affirm; to ensure is to make certain; to insure is to indemnify for money.

He assured me that the work had been completed.

The procedure ensures that clear guidelines have been established.

You cannot get a mortgage unless you insure your home.

Choose “affect”, “effect”, and “impact” depending on your meaning. When “affect” is used as a verb, it means to influence, modify, or change. When “effect” is used as a verb, it means to bring about, but as a noun it means consequence, outcome, or result. “Impact” is a noun meaning a significant effect.

The increased use of pesticides affects agricultural productivity.

The use of polychlorinated benzenes has an effect on the cancer rate.

The effect of the added acid was negligible.

The new procedure effected a 50% increase in yield.

The impact of pesticide use on health is felt throughout the world.

The acid did not have a great impact on the reaction rate.

Use “whether” to introduce at least two alternatives, either stated or implied.

I am not sure whether I should repeat the experiment.

I am not sure whether I should repeat the experiment or use a different statistical treatment.

I am going to repeat the experiment whether the results are positive or negative.

Use “whether or not” to mean “regardless of whether”.

INCORRECT

I am not sure whether or not to repeat the experiment.
CORRECT

I am not sure whether to repeat the experiment.
Whether or not the results are positive, I will repeat the experiment.
Whether or not I repeat the experiment, I will probably leave the laboratory late tonight.

➤ Use “to comprise” to mean “to contain” or “to consist of”; it is not a synonym for “to compose”. The whole *comprises* the parts, or the whole *is composed of* the parts, but the whole is not comprised of the parts. Never use “is comprised of”.

INCORRECT

A book is comprised of chapters.

CORRECT

A book comprises chapters.
A book is composed of chapters.

INCORRECT

Our research was comprised of three stages.

CORRECT

Our research comprised three stages.

**Use of “A” and “An”**

➤ Choose the articles “a” and “an” according to the pronunciation of the words or abbreviations they precede. See pp 257 and 264 for the use of “a” and “an” with chemical elements and isotopes.

- a nuclear magnetic resonance spectrometer
- an NMR spectrometer

➤ Use “a” before an aspirated “h”; use “an” before the vowel sounds of a, e, i, o, “soft” or “short” u, and y.

- a house, a history (*but* an hour, an honor)
- a union, a U-14C (*but* an ultimate)
- a yard (*but* an ylide, an yttrium compound)

➤ Choose the proper article to precede B.A., B.S., M.A., M.S., and Ph.D., according to pronunciation of the first letter.

- a B.S. degree
- an M.S. degree
- a Ph.D.
Words and Phrases To Avoid

➤ Avoid slang and jargon.

➤ Be brief. Wordiness obscures your message and annoys your readers.

➤ Omit empty phrases such as

As already stated
It has been found that
It has long been known that
It is interesting to note that
It is worth mentioning at this point
It may be said that
It was demonstrated that

➤ Omit excess words.

INSTEAD OF
It is a procedure that is often used.
There are seven steps that must be completed.
This is a problem that is ....
These results are preliminary in nature.

CONSIDER USING
This procedure is often used.
Seven steps must be completed.
This problem is ....
These results are preliminary.

➤ Write economically (and usually more precisely) by using single words instead of phrases.

INSTEAD OF
a number of
a small number of
are found to be
are in agreement
are known to be
at present
at the present time
based on the fact that
by means of
despite the fact that
due to the fact that
during that time
fewer in number
for the reason that
has been shown to be
if it is assumed that
in color, e.g., red in color
in consequence of this fact
in length
in order to
in shape, e.g., round in shape
in size, e.g., small in size

CONSIDER USING
many, several
a few
are
agree
are
now
now
because
by
although
because
while
fewer
because
is
if
just state the color, e.g., red
therefore, consequently
long
to
just state the shape, e.g., round
just state the size, e.g., small
Do not use contractions in scientific papers.

**Incorrect**

The identification wasn’t confirmed by mass spectrometry.

**Correct**

The identification was not confirmed by mass spectrometry.

Do not use the word “plus” or the plus sign as a synonym for “and”.

**Incorrect**

Two bacterial enzymes were used in a linked-enzyme assay for heroin plus metabolites.

**Correct**

Two bacterial enzymes were used in a linked-enzyme assay for heroin and its metabolites.

Do not use “respectively” when you mean “separately” or “independently”.

**Incorrect**

The electrochemical oxidations of chromium and tungsten tricarbonyl complexes, respectively, were studied.

**Correct**

The electrochemical oxidations of chromium and tungsten tricarbonyl complexes were studied separately.
Avoid misuse of prepositional phrases introduced by “with”.

**POOR**

Nine deaths from leukemia occurred, with six expected.

**BEST**

Nine deaths from leukemia occurred, and six had been expected.

**POOR**

Of the 20 compounds tested, 12 gave positive reactions, with three being greater than 75%.

**BEST**

Of the 20 compounds tested, 12 gave positive reactions; three of these were greater than 75%.

**POOR**

Two weeks later, six more animals died, with the total rising to 25.

**BEST**

Two weeks later, six more animals died, and the total was then 25.

Do not use a slash to mean “and” or “or”.

**INCORRECT**

Hot/cold extremes will damage the samples.

**CORRECT**

Hot and cold extremes will damage the samples.

Replace “and/or” with either “and” or “or”, depending on your meaning.

**INCORRECT**

Our goal was to confirm the presence of the alkaloid in the leaves and/or roots.

**CORRECT**

Our goal was to confirm the presence of the alkaloid in the leaves and roots.

Our goal was to confirm the presence of the alkaloid in either the leaves or the roots.

Our goal was to confirm the presence of the alkaloid in the leaves, the roots, or both.

If you have already presented your results at a symposium or other meeting and are now writing the paper for publication in a book or journal, delete all references to the meeting or symposium, such as “Good afternoon, ladies and gentlemen”, “This morning we heard”, “in this symposium”, “at this meeting”, and
“I am pleased to be here”. Such phrases would be appropriate only if you were asked to provide an exact transcript of a speech.

➤ Avoid using the word “recently”. Your article or book may be available for a long time. This word will make it look dated in little time.

POOR

It was recently found that these effects enhance the bond strength.

BETTER

Harris and Harris (2006) found that these effects enhance the bond strength.

**Gender-Neutral Language**

The U.S. government and many publishers have gone to great effort to encourage the use of gender-neutral language in their publications. Gender-neutral language is also a goal of many chemists. Recent style guides and writing guides urge copy editors and writers to choose terms that do not reinforce outdated sex roles. Gender-neutral language can be accurate and unbiased and not necessarily awkward.

The most problematic words are the noun “man” and the pronouns “he” and “his”, but there are usually several satisfactory gender-neutral alternatives for these words. Choose an alternative carefully and keep it consistent with the context.

➤ Instead of “man”, use “people”, “humans”, “human beings”, or “human species”, depending on your meaning.

OUTDATED

The effects of compounds I–X were studied in rats and man.

GENDER-NEUTRAL

The effects of compounds I–X were studied in rats and humans.

OUTDATED

Men working in hazardous environments are often unaware of their rights and responsibilities.

GENDER-NEUTRAL

People working in hazardous environments are often unaware of their rights and responsibilities.

OUTDATED

Man’s search for beauty and truth has resulted in some of his greatest accomplishments.

GENDER-NEUTRAL

The search for beauty and truth has resulted in some of our greatest accomplishments.
Instead of “manpower”, use “workers”, “staff”, “work force”, “labor”, “crew”, “employees”, or “personnel”, depending on your meaning.

Instead of “man-made”, use “synthetic”, “artificial”, “built”, “constructed”, “manufactured”, or even “factory-made”.

Instead of “he” and “his”, change the construction to a plural form (“they” and “theirs”) or first person (“we”, “us”, and “ours”). Alternatively, delete “his” and replace it with “a”, “the”, or nothing at all. “His or her”, if not overused, is also acceptable. Using passive voice or second person (“you”, “your”, and “yours”) also works sometimes.

OUTDATED
The principal investigator should place an asterisk after his name.

GENDER-NEUTRAL
Principal investigators should place asterisks after their names.
If you are the principal investigator, place an asterisk after your name.
The name of the principal investigator should be followed by an asterisk.

Do not use a plural pronoun with a singular antecedent.

INCORRECT
The principal investigator should place an asterisk after their name.

CORRECT
The principal investigators should place asterisks after their names.

Instead of “wife”, use “family” or “spouse” where appropriate.

OUTDATED
The work of professionals such as chemists and doctors is often so time-consuming that their wives are neglected.

GENDER-NEUTRAL
The work of professionals such as chemists and doctors is often so time-consuming that their families are neglected.

OUTDATED
the society member and his wife

GENDER-NEUTRAL
the society member and spouse
Electronic submission of manuscripts to journals is undergoing significant change as publishers respond to mounting pressure to publish faster, better, and more efficiently. The use of the Web and e-mail enables the peer-review process to move more rapidly, speeding review and decision cycles. And although scientific research has always been an international activity, journal publishing is increasingly global, with authors, reviewers, and editors contributing from numerous countries and all participants benefiting from electronic communications.

**Reminder:** Good practices and appropriate file creation start early in the manuscript preparation process. If author source files are not of adequate quality for production, then the publication process will be delayed. Authors should be mindful of publishers’ requirements early in the writing process.

This chapter covers the major systems used by dominant commercial publishers and professional societies to manage the submission, review, and acceptance of scholarly manuscripts, and it endeavors to guide authors through the routine tasks associated with submitting a manuscript online. It is important to acknowledge that publishers will revise their systems and add new features quickly, so the information that follows will likely age rapidly. However, authors can rely on this chapter to guide them through the general process of online submission.

Proprietary and commercial editorial systems are frequently designed to accommodate both electronic and paper publication processes. Capabilities vary,
but many systems have become similar as publishers establish parallel mechanisms for managing the peer-review process. Leading commercial software packages currently include Bench>Press from HighWire Press, Editorial Manager from Aries Systems, EJPress from eJournal Press, ScholarOne Manuscript Central, and Rapid Review from Cadmus Systems. Other Web-based commercial products include EdiKit from Berkeley Electronic Press; myICAAP, EPRESS, ESPERE, Fontisworks, and Open Journal Systems from University of British Columbia; PublishASAP; Temple Peer Review Manager; and Xpress Track. Each package provides authors, reviewers, and editors with submission acknowledgments, decision letters, and review documents transmitted using e-mail; no paper correspondence is needed.

Several publishers have opted to develop proprietary programs rather than purchase services from a third party. Examples include the American Chemical Society’s ACS Paragon System and the American Institute of Physics’ Peer X-Press. These packages offer features and workflow similar to those contained in commercial editorial packages.

Appendix 5-1 matches selected scientific publishers and research grant agencies with the manuscript submission software they use and manuscript submission sites.

Preparing Materials

The author guidelines for each journal contain generic and journal-specific instructions concerning manuscript preparation. They indicate the types of components that are required for online submissions, such as the cover letter, abstract, manuscript document, supporting information, figures, and proposed reviewers. Publishers require these items to be submitted in common word-processing or graphics formats, and author guidelines provide the technical details for preparing these manuscript components. Assembling and organizing electronic components of a manuscript in advance will streamline the process and reduce the possibility of errors in submission.

The author guidelines will indicate if there are word-processing templates available for authors to download and will specify if there are requirements about their use. Template files contain all the necessary formatting for a particular journal and are provided by the publisher from its Web site. Templates make it easier to format submissions to meet the publisher’s specifications.

It is important to understand why authors are asked to provide manuscripts as both word-processing and PDF files. These versions of the manuscript are used in different ways; the PDF version of a manuscript is more suitable for peer review because it is easily transferred among authors, editors, and reviewers and is readable with the ubiquitous free Adobe Acrobat Reader. PDF files are portable
across computer platforms, whereas original word-processing files may not be compatible with the system of an editor or reviewer. Publishers may require that authors submit a PDF file, or they may automatically generate one as part of the online submission process. A PDF file assists in maintaining control of versions of the manuscript because editors, authors, and reviewers can insert comments and notes for correction without altering the original text. Most publishers will require word-processing (or TeX or its derivatives) files for production purposes. These versions of the manuscript are manipulated during the final electronic creation of a journal for publication online or in print.

**Reminder:** Most publishers require both PDF and word-processing versions of a manuscript to be used for peer review and publication production, respectively.

Another critical element of your submission is the figures associated with the manuscript. Graphics should be high-resolution and of good quality to ensure clarity and accuracy in the final published copy and to facilitate any needed reduction required in the print publication (see Chapter 15 for more detail on preparing illustrations). Many software programs—including PowerPoint, Word, Excel, and WordPerfect—do not create high-resolution images suitable for publication. For that reason, it is recommended that authors create graphics using applications that can prepare figures in TIFF or EPS formats. Figures should have clear, sharp lines, should be clearly labeled, and should be at a high enough resolution that they can be used to compose the print journal.

Appendix 5-2 presents the text and image formats accepted by seven major manuscript peer-review and submission systems.

**Beginning Your Submission**

Depending on the publisher, authors may be asked to e-mail the prepared manuscript to the editor, to upload it via an FTP server, or to upload files through the publisher’s Web browser to a secure Web site using HTTP protocol. It is extremely important to submit manuscripts in the method designated for that particular journal because submission mechanisms may vary, even within one publisher’s journals. If the journal requires online manuscript submission, submit all files to that Web site. Similarly, if the journal uses FTP or e-mail, follow the instructions carefully and send all manuscript components via the same route, unless indicated otherwise.

When authors are asked to e-mail the manuscript directly to an editor, pay particular attention to the type of files authors are asked to provide, and note
if the manuscript should be provided in the body of the e-mail or as an attachment. Publishers offering an FTP server for author use will have detailed instructions on how to access the FTP server. Authors may be asked to compress files when transmitting manuscripts by e-mail, FTP, or as part of an online submission system. If so, the publisher’s Web site will detail the acceptable formats for compressed files. These may include zipped, tarred, uuencoded, or BinHex files. Under some circumstances, Web uploads will automatically invoke a compression process.

Leading online submission packages Bench>Press, Editorial Manager, EJPress, Manuscript Central, and Rapid Review, as well as the ACS Paragon System and the American Institute of Physics’ Peer X-Press all use the author home page. This simple online profile contains the author’s contact details and establishes a user name and password. The e-mail address entered here must be correct; a typo could delay important e-mail notifications about acceptance or requests for revision. If the author has already established an account, future submissions can begin with the author login.

Several publishers have adopted the concept of a submitting agent or a second author if someone other than the author is submitting the manuscript on the author’s behalf. This person is responsible for the tasks associated with submission, but correspondence and requests for further changes are made to the party designated as the corresponding or primary author of the manuscript. Submitting agent accounts are created similarly to author accounts, but they require information about the primary author also to be added to the user account profile.

Passwords to either author accounts or submitting agent accounts should not be shared. Doing so leaves the account holder at risk of incomplete submissions being changed or new submissions being created under his or her name.

The Author Home Page

After logging in, the author is presented with his or her home page. Typically, the author home page is divided into several areas; from this location, authors can begin a new submission, check the status of a previous submission, continue a submission begun earlier, or submit a revised manuscript. The author home page also shows the progress of accepted manuscripts through the production cycle to publication. As publishers increasingly recognize the value of this author home page, new features are likely to be added. In the case of the Cadmus Rapid Review software, the author home page has already evolved to include a scientist’s activities as both a referee and an author.

Reminder: If an author home page is available, use it to submit new articles and to track the status of current submissions.
Submitting Your Manuscript

Preparing materials in advance allows the authors either to complete their full submissions in one sitting or to partially complete the process, depending on individual preferences and the requirements of the publisher. E-mail and FTP submissions require the submission to be completed at one time. However, more publishers with online submission sites allow authors to interrupt their online submissions and to complete them later. During a partial submission, each step must be completed for the information pertaining to that submission step to be saved. The author can complete the submission by logging into the journal site and accessing his or her author home page. After selecting the link for that manuscript, the submission process can be resumed, beginning with the first incomplete step. Before the manuscript is submitted, authors are asked to review all the component parts and make any final changes.

Supplemental information should also be reviewed and validated. Crystallographic information files (CIFs) in particular can be verified using the free CheckCIF utility, which is available from the International Union of Crystallography.

Usually in the cases of e-mail, FTP, or online submission, no additional changes to the manuscript or associated documents are permitted after submission unless an editor requests a revision or the publisher contacts the author to fix a problem.

Submitted Manuscripts

After the submission is complete, the author typically receives an e-mail acknowledging the submission from either the editor or the submission system. If the publisher offers an author home page, the status of the manuscript can be tracked from that site. These sites also notify authors by e-mail as the status of the manuscript changes. If the publisher makes use of an online system for submission, the editors for that publisher may be able to use features available only to them to shepherd the manuscript through the peer-review process. In these cases, the system notifies the editor of newly arrived manuscripts, allows the editor to view all associated files and details of the submission, and allows for the manuscript to be assigned to the appropriate editors and reviewers. Many systems generate the correspondence that accompanies the notification of editors, reviewers, and authors. As decisions are made and correspondence is sent, the corresponding status changes for the manuscript are displayed on the author home page. Additional details about the peer-review process can be found in Chapter 6.

Stops Along the Way (Revisions)

When a revision of the paper is requested, an e-mail from the editor will detail the necessary changes. Where FTP or direct-to-editor e-mail is the preferred sub-
mission mechanism, the author will send revised files directly to the indicated e-mail address or FTP location. For publishers with author home pages, authors can view the status of submitted manuscripts and determine that a revision has been requested. From the author home page, authors access the submission and upload revised manuscript documents, images, and associated files. During the submission of the revision, authors may also provide rebuttal information or revision details to clarify how the manuscript has been altered. If an author determines that a revision is necessary before a request is made by the editor, authors using Web-based submission systems must contact the appropriate editor and request that the status of the manuscript be changed within the system to indicate that a revision is needed. This step will allow the author to adjust and replace files and then to submit a revision. Once the revision is received, an acknowledgment is sent by e-mail, and the author will not be able to make further changes to the paper unless the editor requests another revision to the manuscript.

Acceptance

Authors can expect to be notified of their manuscripts’ acceptance by e-mail. Accepted manuscripts are copyedited and formatted according to specific journal style, using the original word-processing files from the author’s online submission. As the manuscript progresses through the various stages of production, the status on the author home page changes to reflect each new step.
APPENDIX 5-1
Online Submission at Selected Scientific Publishers and Research Grant Agencies

This appendix contains a list of scientific publishers and research grant agencies, along with the software they use for online manuscript submission and the manuscript submission site, if there is one.

Table 5A-1. Scientific Publishers

<table>
<thead>
<tr>
<th>Publisher</th>
<th>Software</th>
<th>URL</th>
</tr>
</thead>
<tbody>
<tr>
<td>American Academy of Forensic Science</td>
<td>Information and forms only</td>
<td>No electronic submission</td>
</tr>
<tr>
<td>American Association for Clinical Chemistry</td>
<td>Bench&gt;Press</td>
<td><a href="http://submit.clinchem.org/?ctst=y">http://submit.clinchem.org/?ctst=y</a></td>
</tr>
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</tr>
<tr>
<td>American Geophysical Union</td>
<td>Geophysical Electronic Manuscript System</td>
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</tr>
<tr>
<td>American Institute for Chemical Engineers</td>
<td>Rapid Review</td>
<td><a href="https://www.rapidreview.com/AICheE/CALogon.jsp">https://www.rapidreview.com/AICheE/CALogon.jsp</a></td>
</tr>
<tr>
<td></td>
<td></td>
<td>After acceptance, you will be asked to use their FTP or e-mail site at <a href="http://www.aip.org/epub/submittext.html">http://www.aip.org/epub/submittext.html</a>.</td>
</tr>
<tr>
<td>American Mathematical Society</td>
<td>Information and forms only</td>
<td>No electronic submission</td>
</tr>
<tr>
<td>American Peptide Society</td>
<td>ScholarOne Manuscript Central</td>
<td><a href="http://bip-pep-wiley.manuscriptcentral.com/">http://bip-pep-wiley.manuscriptcentral.com/</a></td>
</tr>
<tr>
<td>American Physical Society</td>
<td>—</td>
<td><a href="http://publish.aps.org/ESUB/">http://publish.aps.org/ESUB/</a></td>
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Continued on next page
### Table 5A-1. Scientific Publishers—Continued

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<tr>
<td>American Society for Microbiology</td>
<td>Rapid Review</td>
<td><a href="https://www.rapidreview.com/ASM2/Calogon.jsp">https://www.rapidreview.com/ASM2/Calogon.jsp</a></td>
</tr>
<tr>
<td>Biophysical Society</td>
<td>Bench&gt;Press</td>
<td><a href="http://submit.biophysj.org/?ctst=y">http://submit.biophysj.org/?ctst=y</a></td>
</tr>
<tr>
<td>Blackwell Publishing</td>
<td>Information and forms only</td>
<td>No electronic submission</td>
</tr>
<tr>
<td>Cambridge University Press</td>
<td>Information and forms only</td>
<td>No electronic submission</td>
</tr>
<tr>
<td>Elsevier</td>
<td>Elsevier author gateway</td>
<td>Each journal has its own instructions for submitting work. Go to the home page of your journal of interest at <a href="http://authors.elsevier.com/">http://authors.elsevier.com/</a>.</td>
</tr>
<tr>
<td>Institute of Electrical &amp; Electronics Engineers (IEEE)</td>
<td>—</td>
<td>Each journal has its own instructions for submitting work. Go to the home page of your journal of interest at <a href="http://www.ieee.org/organizations/pubs/guide.html">http://www.ieee.org/organizations/pubs/guide.html</a>.</td>
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<tr>
<td>Oxford University Press</td>
<td>Some journals use ScholarOne Manuscript Central</td>
<td>Each journal has its own instructions for submitting work. Go to the home page of your journal of interest at <a href="http://www3.oup.co.uk/jnls/">http://www3.oup.co.uk/jnls/</a></td>
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<tr>
<td>Royal Society of Chemistry</td>
<td>ReSourCe</td>
<td><a href="http://chemistry.rsc.org/Publishing/ReSourCe/">http://chemistry.rsc.org/Publishing/ReSourCe/</a></td>
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<tr>
<td>Science</td>
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<tr>
<td>Society of Plastics Engineers</td>
<td>Information and forms only</td>
<td>No electronic submission</td>
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<td>Society of Toxicology</td>
<td>ScholarOne Manuscript Central</td>
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<tr>
<td>Taylor &amp; Francis</td>
<td>Information and forms only</td>
<td>No electronic submission</td>
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<td>Wiley-VCH</td>
<td>Some journals use ManuscriptXpress</td>
<td>Each journal has its own instructions for submitting work. Go to the home page of your journal of interest.</td>
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<tr>
<td>World Scientific</td>
<td></td>
<td>Each journal has its own instructions for submitting work. Go to the home page of your journal of interest at <a href="http://www.worldscinet.com/subject.shtml">http://www.worldscinet.com/subject.shtml</a>.</td>
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Table 5A-2. Research Grant Agencies

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<td>No electronic submission <a href="http://www.humboldt-foundation.de/en/programme/bewerbung.htm">http://www.humboldt-foundation.de/en/programme/bewerbung.htm</a></td>
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<td>American Chemical Society Petroleum Research Fund</td>
<td>—</td>
<td>Electronic submission only. <a href="http://www.chemistry.org/prf">http://www.chemistry.org/prf</a></td>
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<tr>
<td>Australian Research Council</td>
<td>Grant Application Management System (GAMS)</td>
<td>Electronic submission only. <a href="https://gams.arc.gov.au/">https://gams.arc.gov.au/</a></td>
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<tr>
<td>Camille and Henry Dreyfus Foundation</td>
<td>Limited online submission</td>
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<td>Ford Foundation Diversity Fellowships</td>
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<tr>
<td>The National Academies, Research Associateship Programs</td>
<td>NRC WebRAP</td>
<td><a href="http://nrc58.nas.edu/nrcwebrap/rap/login/Register.asp">http://nrc58.nas.edu/nrcwebrap/rap/login/Register.asp</a></td>
</tr>
<tr>
<td>National Institutes of Health, Office of Extramural Research</td>
<td>Information and forms only</td>
<td>No electronic submission <a href="http://grants1.nih.gov/grants/oer.htm">http://grants1.nih.gov/grants/oer.htm</a></td>
</tr>
<tr>
<td>National Science Foundation</td>
<td>FastLane</td>
<td><a href="https://www.fastlane.nsf.gov/fastlane.jsp">https://www.fastlane.nsf.gov/fastlane.jsp</a></td>
</tr>
<tr>
<td>Office of Naval Research</td>
<td>Information only</td>
<td>No electronic submission <a href="http://www.onr.navy.mil/02/how_to.asp">http://www.onr.navy.mil/02/how_to.asp</a></td>
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<tr>
<td>proposalCENTRAL</td>
<td>Research and Management System (RAMS)</td>
<td><a href="https://v2.ramscompany.com/">https://v2.ramscompany.com/</a></td>
</tr>
<tr>
<td>Welch Foundation</td>
<td>Information and forms only</td>
<td>No electronic submission <a href="http://www.welch1.org/">http://www.welch1.org/</a></td>
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<tr>
<td>Wellcome Trust</td>
<td>eGrants</td>
<td><a href="http://www.wellcome.ac.uk/node2110.html">http://www.wellcome.ac.uk/node2110.html</a> or <a href="http://www.wellcome.ac.uk/doc_WTD004053.html">http://www.wellcome.ac.uk/doc_WTD004053.html</a></td>
</tr>
</tbody>
</table>
APPENDIX 5-2

Key Features of Selected Online Submission Systems

The following systems are entirely Internet-based and incorporate all elements of submission, review, and manuscript management, unless otherwise noted. They operate with standard browsers and require that authors, editors, and reviewers have Adobe Acrobat Reader to view PDF documents. Authors, reviewers, and editors are offered a secure, password-protected login. Each system incorporates an author home page for the submission, revision, and tracking of manuscripts. Similarly, each system allows referees to submit reviews of manuscripts online.

Publishers modify these systems in varying degrees to reflect different workflows. For this reason, journals using the same software may have slightly different features. This list indicates acceptable submission file types for each system and highlights the system’s distinctive features. As technology changes and new features become available, publishers will amend submission sites and systems. Therefore, authors should check regularly for current requirements with the journal before beginning a manuscript submission.

Table 5A-3 catalogs a variety of scientific publishers and the systems they currently use to accept manuscripts online. This table is not all-encompassing, but it is intended to be representative of publishing organizations that contribute to the peer-review literature used by ACS members.
## Table 5A-3. Text and Image Formats Acceptable to Different Web-Based Manuscript Submission Systems

<table>
<thead>
<tr>
<th>Format</th>
<th>ACS Paragon System</th>
<th>Bench&gt;Press</th>
<th>Editorial Manager</th>
<th>EJPress</th>
<th>Manuscript Central</th>
<th>Peer X-Press</th>
<th>Rapid Review</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Text Formats</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MS Word (.DOC)</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>—</td>
</tr>
<tr>
<td>WordPerfect (.WPD)</td>
<td>—</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>—</td>
</tr>
<tr>
<td>Encapsulated PostScript (.EPS)</td>
<td>Yes</td>
<td>—</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
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</tr>
<tr>
<td>PostScript (.PS)</td>
<td>Yes</td>
<td>—</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>—</td>
</tr>
<tr>
<td>Text—ASCII (.TXT)</td>
<td>—</td>
<td>—</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>Rich text format (.RTF)</td>
<td>Yes</td>
<td>—</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>—</td>
</tr>
<tr>
<td>TeX</td>
<td>Yes</td>
<td>—</td>
<td>Yes</td>
<td>—</td>
<td>Yes</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>LaTeX</td>
<td>Yes</td>
<td>—</td>
<td>Yes</td>
<td>—</td>
<td>Yes</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>Portable document format (.PDF)</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
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</tr>
<tr>
<td><strong>Image Formats</strong></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>Graphics interchange format (.GIF)</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
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</tr>
<tr>
<td>Joint Photographic Experts Group (.JPEG)</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
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</tr>
<tr>
<td>Tagged image file (.TIF)</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>—</td>
</tr>
<tr>
<td>Encapsulated PostScript (.EPS)</td>
<td>—</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>PostScript (.PS)</td>
<td>—</td>
<td>—</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
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<tr>
<td>MS PowerPoint (.PPT)</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>Yes</td>
<td>—</td>
</tr>
<tr>
<td><strong>Other Acceptable Formats</strong></td>
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<td></td>
<td></td>
<td></td>
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<td></td>
</tr>
<tr>
<td>Chemical markup language (.CML)</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>—</td>
<td>Yes</td>
<td>—</td>
<td>Yes</td>
</tr>
<tr>
<td>Chemical structures, such as those created by ChemDraw, ChemSketch, ISIS/Draw</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>—</td>
<td>Yes</td>
<td>—</td>
<td>Yes</td>
</tr>
<tr>
<td>DrawIt (formerly Chemwindow)</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>—</td>
<td>Yes</td>
<td>—</td>
<td>Yes</td>
</tr>
<tr>
<td>Crystallographic information file (.CIF)</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>—</td>
<td>Yes</td>
<td>—</td>
<td>Yes</td>
</tr>
<tr>
<td>Executable (.EXE)</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>—</td>
<td>Yes</td>
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<td>Yes</td>
</tr>
<tr>
<td>MS Excel (.XLS)</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>—</td>
<td>Yes</td>
<td>—</td>
<td>Yes</td>
</tr>
<tr>
<td>MOL</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>—</td>
<td>Yes</td>
<td>—</td>
<td>Yes</td>
</tr>
<tr>
<td>Video files, such as QuickTime (.AVI, .MPEG)</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>—</td>
<td>Yes</td>
<td>—</td>
<td>Yes</td>
</tr>
<tr>
<td>Protein Data Bank (.PDB)</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>—</td>
<td>Yes</td>
<td>—</td>
<td>Yes</td>
</tr>
<tr>
<td>Windows metafile (.WMF)</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>—</td>
<td>Yes</td>
<td>—</td>
<td>Yes</td>
</tr>
<tr>
<td>Winzip file (.ZIP)</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>—</td>
<td>Yes</td>
<td>—</td>
<td>Yes</td>
</tr>
</tbody>
</table>

Note: The systems and their developers are as follows: ACS Paragon System, American Chemical Society; Bench>Press, HighWire Press; Editorial Manager, Aries Systems; EJPress, eJournal Press; Manuscript Central, ScholarOne; Peer X-Press, American Institute of Physics; and Rapid Review, Cadmus Systems.

a These systems allow a variety of designated file types to be uploaded as supplemental information.

b These systems allow any file type to be uploaded as supplemental information.
Peer review is a process used by scientific publications to assist editors in evaluating manuscripts, particularly for scientific merit. It is not the only system used to evaluate manuscripts, and it is not perfect. Editors of peer-reviewed books and journals send manuscripts to several reviewers and request their opinions on originality and scientific importance of the topic, the quality of the work performed, and the appropriateness for the specific journal. Reviewers may also comment on language usage, clarity of figures and tables, manuscript length, and anything that they find relevant to effective communication. Although not every editor uses peer review in the same manner, this chapter presents a summary of many common attributes of the peer-review process. (For a broader discussion of peer review, see “Peer Review and the Acceptance of New Scientific Ideas” at http://www.senseaboutscience.org.uk/PDF/peerReview.pdf.)

Purpose of Peer Review

When a manuscript is submitted for consideration, peer review provides the editor with advice on whether to accept the manuscript for publication. Reviewers also provide suggestions for improving the manuscript. The decision on whether to accept the manuscript for publication rests solely with the editor. Reviewers provide additional expertise and have perspectives that may complement that of the editor. Customarily, peer review is anonymous: the identities of reviewers are not revealed by editors. Some journals also hold authors’ names and affiliations in confidence, a double-blind review approach. Occasionally, reviewers request...
that the editor disclose their names to authors; this is allowed at the discretion of the editor, based on the policy of the individual publication. In one variation of the peer-review process, review is not anonymous; all reviewers are identified.

Peer review is also intended to help authors. External review can help improve the presentation and interpretation of data alike, and ultimately, the research. Clearly and succinctly describing a scientific study is challenging, and reviewers provide valuable feedback. Few manuscripts are so well written that they are accepted without revision. Data and interpretation that seem clear to authors are not always comprehensible to readers. Scientific research is both competitive and cooperative; at its best, peer review is a part of the cooperative process. For example, after evaluating data, a reviewer may suggest an alternative explanation or additional experiments that trigger ideas for further research. Also, a reviewer pointing out an error can save an author the embarrassment of subsequently publishing a correction.

**The Peer-Review Process**

When the editor receives a manuscript, he or she examines it and determines whether the manuscript fits within the scope of the journal, whether it meets the specific requirements of the journal, and whether it is of sufficient scientific merit for consideration. Not all manuscripts are transmitted to reviewers. In some cases, the editor decides to reject a manuscript without review, or rarely, to accept it for publication. Manuscripts are rejected without review for various reasons, including the following: the topic is inappropriate for the journal; the concept or the data are not novel; the format is incorrect; the writing is so poor that the manuscript is unreadable; or the authors have previously published overly similar papers. If a manuscript is rejected without review, the editor will usually briefly inform the author of the reason. Some editors offer suggestions to help authors with future submissions.

If the editor decides to send the manuscript for peer review, customarily two to four individuals with appropriate expertise—training or research experience—are asked to review the manuscript. The editor may identify reviewers in a number of ways. Many editors ask authors to recommend reviewers; some do not. Author-recommended reviewers may or may not be used. Most editors will not send manuscripts to specific reviewers if an author so requests. Other potential reviewers may be authors cited in the manuscript, acknowledged experts in the field, or other active researchers in the field. Editors often use scientific search services (such as SciFinder or SciFinder Scholar for chemists) to identify qualified potential reviewers. Reviewers may or may not be known personally to the editor. Most journals maintain records on thousands of reviewers, including their expertise, manuscripts they have reviewed, performance, and so on.
Usually, reviewers are asked whether they are willing to review a manuscript. If they agree, the manuscript is provided in either hard copy or electronically, often with an accompanying review form. Editors generally ask reviewers to submit their reviews in two or three weeks. When a review is overdue, the editor usually sends a reminder to the reviewer.

Once reviews are returned, the editor reads the reviews in conjunction with the relevant manuscript, evaluating both the manuscript and the reviews, and then makes a decision whether to accept the manuscript, request revisions, reject the manuscript, or send it for additional review. In some cases of conflicting advice or opinions of reviewers, editors may seek advice from others. Editors are not obligated to follow the recommendations of reviewers. Reviewer ratings are not averaged; often, a single cogent negative review leads to rejection of a manuscript.

Responsibilities of Reviewers

Peer review is a critical component of formal scientific communication, and every scientist has an obligation to do a fair share of reviewing.

Reminder: Manuscripts should be reviewed in a timely and balanced manner and should be kept confidential until publication.

When a manuscript is under review, it is a confidential document and it should not be discussed or shown to others. After reading a manuscript, a reviewer may conclude that a better review could be accomplished with assistance from a colleague. In this circumstance, the reviewer should inform the editor before engaging the colleague. Reviewers are expected to provide reviews that are thorough and unbiased. A reviewer in direct competition with the authors of a manuscript should inform the editor that there is a potential conflict of interest and discuss the issue with the editor. In addition, if reviewers are asked to review the work of someone at the same institution or the work of a previous student or co-worker, the reviewer should inform the editor. In some cases, the editor will excuse the reviewer from doing the review; in other cases, the editor will consider the relationship when evaluating the review.

Reviewers are expected to submit their reviews on time. Most reviewers are also authors and expect reviews of their manuscripts to be handled expeditiously. If circumstances arise that prevent or delay a review, the editor should be informed as soon as possible.

The entire manuscript should be read carefully and critically. Most reviewers read a manuscript more than once. Manuscripts should be rated on technical quality, significance of the work, importance to the research field, and adequacy of expression. Often a standard form is provided for this portion of the review.
The ACS Style Guide

Reviewers should feel free to comment on the suitability of the manuscript for the particular publication. Sometimes first-rate manuscripts are submitted to an inappropriate publication. In addition to the actual review, some editors allow reviewers to submit confidential comments about the manuscript. These are not forwarded to the author. If suspicions of abuse, plagiarism, or fraud arise, the editor should be informed immediately.

Many reviewers divide their reviews into general comments and specific, detailed comments. In the general section, reviewers should draw attention to both the strong and the weak points of the manuscript, the concepts, the objectives, and the methods. Like an author writing a manuscript, reviewers should write reviews in a comprehensive but concise manner, addressing the questions presented in Box 6-1.

Reviews should be written in a helpful, tactful manner. Editors generally edit or do not pass discourteous comments to authors. Abusive reviews lack credibility and also reflect poorly on the reviewer.

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Box 6-1. Suggested Topics for a Peer Review

- Are the methods (experimental section) adequately described and referenced?
- Are there any unsupported conclusions?
- Is there anything that is confusing or ambiguous?
- Do figures and tables appropriately illustrate the data?
- Is the introduction clear and informative?
- Is either the introduction or discussion longer than necessary, and do they make sense in relation to the subject and the data?
- Although the discussion is the appropriate place for speculation, is it excessive?
- Are the appropriate references cited? Are the references accurate?
- Is English usage and grammar adequate? Some reviewers may be inclined to edit or annotate the manuscript. However, reviews are more valuable to editors if reviewers mention that there are problems with the English and concentrate on evaluating the data and its interpretation.
- Is the length of the manuscript unwarranted? Suggestions on how a manuscript can be shortened are appreciated by editors.
- Is the use of color warranted? Printing color is a significant expense for the publisher.
Responsibilities of Authors

Authors should read the current instructions to authors for the publication to which they intend to submit a manuscript. For journals, these instructions are typically published in the first issue of the year and can often be found on the Web. Author guidelines for books are available from the publisher, and sometimes they are posted on the publisher’s Web site. Many submissions are rejected without review because the manuscript does not conform to the publication guidelines.

Reminder: Authors should read the current instructions to authors for any publication to which they intend to submit a manuscript.

If English is not the author’s native language, it is a good idea to ask a native English speaker to edit the manuscript before submission. Alternatively, authors can employ a technical editing service. Such editing services can be found through recommendations from colleagues, by searching the Web, or advertised in scientific publications. However, it is the author’s responsibility to ensure that the writing is accurate.

In suggesting potential reviewers, authors should not recommend members of their own institution or current or recent collaborators (including students or postdoctoral associates). Many authors suggest the names of eminent scientists in their fields. These individuals are frequently asked to review a large number of manuscripts and, constrained by time, may not be available to review additional manuscripts. Therefore, it is more helpful to suggest the names of highly qualified, less well known researchers. Many book and journal editors also allow authors to request that certain individuals, such as those in direct competition, not be selected to review. Editors usually comply with these requests.

Authors should read reviews carefully and dispassionately, with the expectation that reviewers’ comments will improve their manuscripts. When an editor requests a revision, authors should respond to all comments and answer all questions. Editors generally reject perfunctory revisions. When it is apparent that a reviewer has misread or misinterpreted the text, authors should provide a direct but tactful reply. Revisions should be submitted in a timely manner. Generally, editors expect revisions within a few weeks, not months. If there is long delay in submitting a revision, some editors will consider the revision to be a new manuscript. Sometimes an editor or reviewer will ask authors to perform additional experiments or to reanalyze data, necessitating a delay in submitting a revision. Authors should ask the editor for an extension, if necessary, providing an explanation.

When a manuscript is rejected, authors should read the editor’s letter and reviews carefully to determine the reasons for the rejection. Rejection usually
means that another publication should be considered for submission of the manuscript. Some manuscripts should be abandoned. Although some editors will consider an appeal of a rejection, successful appeals are rare. Only if authors are confident that with the help of the reviews, the research and its presentation can be improved, should they resubmit the manuscript to the same publication. A cover letter accompanying the revision of the rejected manuscript should describe all changes to the manuscript, reply to all reviewer comments, and respond to all questions. Ultimately, whether the manuscript is submitted to a different publication, revised and resubmitted to the same publication, or further experiments are performed to broaden the scope of the investigation, critical assessment from reviewers can aid both research and its communication.

Encouragement to New Investigators

The peer-review process may seem daunting and at times unfair to new investigators. On occasion, reviewers will be unduly critical and unhelpful—and infrequently, outright nasty and rude. Sometimes reviewers can be exasperatingly slow. Good manuscripts are rejected, in particular by prestigious journals, which receive many more high-quality manuscripts than they can publish. However, many reviewers and editors will be solicitous and encouraging to investigators in the early stages of their careers. Despite its shortcomings, peer review is regarded by the scientific community as an essential component to high-quality, effective communication that further advances science.

Reminder: Frequently consult the “Ethical Guidelines to Publication of Chemical Research” (Appendix 1-1 in this book, or on the Web at https://paragon.acs.org). The guidelines are reviewed regularly to ensure their clarity.
Copyright Basics

Karen S. Buehler, C. Arleen Courtney, and Eric S. Slater

Copyright law is a cornerstone of intellectual and scientific exchange. This chapter is intended to introduce a complex and constantly changing legal area; we do not intend to provide legal advice. The first section is an overview of U.S. copyright law: what materials are subject to copyright, who owns copyright, and when copyrighted materials may be used by others. The second part of the chapter presents the methods of obtaining permission to use someone else’s copyrighted work. The third part briefly explains how copyright is transferred from the author to the publisher.

U.S. Copyright Law

What Can Be Copyrighted

Copyright is a doctrine of federal law (Title 17, U.S. Code) and is defined as a form of intellectual property law that protects original works of authorship fixed in a tangible medium of expression for a specified period of time. A tangible medium of expression is something that can be seen, touched, or heard (see the examples below). Copyright applies to all media of expression, including print, the Internet, CD-ROM, and videotape. Copyright allows authors and creators certain rights to protect their original works. Copyright law protects both published and unpublished works.

The authors wish to thank Barbara F. Polansky and William J. Cook for their time in reviewing and commenting on this chapter.
Copyright applies to a variety of works including the following:

- literary works (including scientific works and computer programs);
- musical works (including lyrics);
- dramatic works (including accompanying music);
- pantomimes and choreographic works;
- pictorial, graphic, and sculptural works;
- motion pictures and other audiovisual works;
- sound recordings;
- architectural works; and
- compilations and databases to the extent that they reflect originality in the selection and arrangement of elements.

**What Cannot Be Copyrighted**

Copyright does not protect the following:

- Works not fixed in a tangible form of expression. Copyright does not protect ideas, only the fixed expression of ideas. Thus a thought, not written down in any way, is not protected.
- Titles, names, short phrases, slogans, familiar symbols, or designs. (These items may be protected under trademark or service mark laws.)
- Lists of ingredients, contents, or facts.
- Ideas, procedures, methods, systems, processes, concepts, principles, discoveries, and devices. (These items may be protected under patent law.)
- Standard calendars, rulers, lists, or tables taken from the public domain and other works containing no original authorship.

**Who Owns the Copyright**

The copyright owner is the author or creator of the original work. An original work can be in the form of an article, photograph, illustration, figure, table, etc. Copyright does not protect ideas, only the actual expression of the ideas. Therefore, the copyright owner is the person who drew a figure or table on a computer and saved it, or took a photograph (the subject of the picture is not the copyright owner), or wrote a narrative on a piece of paper.

There are two exceptions when the author or creator of the original work is not the copyright owner: (1) when the copyright was transferred in writing to another person or entity (usually via a copyright status form) and (2) when the work was created as a work-made-for-hire. In a work-made-for-hire situation, employees create the work within the scope of their employment; therefore, the copyright owner is the employer. The employer may be an individual, corporation, or university. The above two examples represent typical scenarios when publishing scientific or scholarly works. Work-made-for-hire can also cover, among other specified categories, independent contractor situations under certain conditions and if the parties have agreed in writing.
Rights of the Copyright Owner

The copyright owner can be described as controlling a “bundle” of stated rights. The copyright owner (whether an individual, a corporation, or a publisher) retains certain exclusive rights in the work. The bundle of rights includes

- reproducing copies of the work;
- distributing copies of the work to the public;
- creating derivative works based on the work;
- performing the work publicly (for certain types of works) and, in the case of sound recordings, by digital audio transmission; and
- displaying the work publicly (for certain types of works).

Most scientific and scholarly publishers require authors (or their employers) to transfer copyright as part of their publication agreement. The ACS Publications Division requires authors (or their employers) to transfer copyright to the American Chemical Society, although some rights are transferred back to the authors (or their employers). For specific information regarding transferring copyright to ACS and authors’ rights, see http://pubs.acs.org/copyright_info.html or contact the ACS Copyright Office (see Box 7-1).

Copyright Notice

A work is protected by copyright even if it does not contain a formal copyright notice (the word “copyright”, abbreviation “copr”, or symbol © with the year of first publication and name of copyright owner). It is strongly recommended to place a copyright notice in or on a work, thereby giving notice that someone controls the rights to that work. Registration of a work with the U.S. Copyright Office is not necessary to obtain copyright protection, although there are substantial
benefits to doing so. For more information about copyright registration, contact the U.S. Copyright Office at 202-707-5959, or at http://www.copyright.gov/.

The U.S. copyright law also provides remedies for infringement. Authors should contact the appropriate book or journal editor in cases where they believe their work has been infringed upon. If a copyright owner (in the case of an ACS publication, the ACS) believes that his or her work has been infringed upon, it is the responsibility of the copyright owner to bring action.

**Fair Use**

The U.S. copyright law contains limitations on rights granted to the copyright owner. Probably one of most misunderstood of these limitations is fair use. Essentially, fair use permits certain actions that might otherwise infringe upon an exclusive right of the copyright owner. It has been our experience that the interpretation of what constitutes fair use can vary widely. For instance, a copyright owner’s interpretation may be very narrow; a party looking to take advantage of fair use will interpret it broadly.

Using excerpts from works for the following purposes may qualify as fair use:

- criticism or comment;
- news reporting;
- teaching (but only in a spontaneous situation. If one knows in advance that copyrighted material will be used in a class, permission must be obtained.); and
- scholarship or research. (Private researchers and nonprofit employees may make one photocopy of an article for their own research purposes only.)

These uses may not constitute copyright infringement. The determination of whether a use is fair depends on the facts in each case. Even if the facts are virtually identical, one degree of minutiae can cut against fair use.

The U.S. copyright law provides four factors that must be considered in determining whether any particular use is fair use. Courts weigh the four factors against each other, and no one factor is determinative in every case. The four factors are the following:

1. the purpose and character of the use, including whether it is of a commercial nature or for nonprofit educational purposes;
2. the nature of the work;
3. the amount and substantiality of the portion used in relation to the work as a whole; and
4. the effect of the use in question on the potential market for or value of the work.

There are no numerical guidelines or percentages that can be used for each situation where fair use might be involved. Even one percent of a work used in a
manuscript may be determined to be against fair use if the material is considered the most important part or the heart of that work. Fair use is a defense, and a strong argument must be made that the use is actually fair. Never assume that a use is a fair use; it is always best to seek permission to avoid potential and sometimes costly problems.

Reminder: Never assume that a use is a fair use; it is always best to seek permission to avoid potential problems.

Public Domain and U.S. Government Works

Works that are in the public domain are not protected by copyright. The following are situations in which a work can have public domain status:

1. works published before 1923 whose copyright term has expired (see the section called “Duration of Copyright”), or works for which copyright was not renewed;
2. works published before 1978 without a proper copyright notice;
3. works dedicated to the public domain by their creator, e.g., so-called shareware; and
4. works authored by U.S. government employees within the scope of their employment.

Generally, it is not necessary to seek anyone’s permission to use public domain works. However, when using material that appeared in a U.S. government publication, check the caption or reference section to see if credit is given to a source for which permission is required.

Reminder: Even though material in a U.S. government publication generally does not require permission to reproduce it, sometimes government publications include material that is protected by copyright. Always check the caption or reference section to determine whether you need to obtain permission to reproduce it.

Common Misconceptions about Copyright

One misconception about copyright status involves material found on Internet Web sites. Someone does own copyright to the material on a Web site, and it is necessary to obtain permission to reuse it. The lack of a copyright notice does not mean that the work is not protected, nor does it mean that a work is in the public domain or that the author of the work has waived his or her rights.

Other misconceptions involve photographs. The individuals appearing in photographs are not the copyright owners. The photographer, or employer if
the photo is a work-made-for-hire, is the copyright owner, and permission to reuse a photograph must come from the copyright owner. (Permission of people appearing in photographs may also be required by a publisher, but this is not a copyright issue. It is a privacy/right of publicity concern.)

Another problem involves the use of photographs of old works of art. It may be true that the art itself is in the public domain (i.e., a van Gogh or Michelangelo painting). However, the photograph of the artwork is protected by copyright. In these cases, the copyright owner may not be an individual photographer but a museum or a historical society.

**Duration of Copyright**

Under current U.S. copyright law, length of copyright is life of the author plus 70 years. For works-made-for-hire, length of copyright is 95 years from the date of first publication, or 120 years from the date of creation, whichever is shorter.

**Copyright in the Electronic Age**

Several recent court cases have involved copyright infringement in electronic media. The legal disputes centered on which party controlled specific rights under the contractual arrangements authors had with publishers. A common thread to these cases is whether a publisher controls all rights to publish content in any format.

Publishers and authors need to be aware of the rights they hold, either explicitly under the U.S. copyright law, or via a licensing arrangement. ACS requires complete transfer of copyright in all formats, thus allowing ACS to publish material in different formats.

In cases where authors do not transfer copyright, publishers generally require a *nonexclusive* licensing arrangement. Here, the author retains copyright and grants certain rights to the publisher. Placing material on the Internet without authorization from the copyright owner is a copyright infringement, even if the publisher had permission to use the material in print.

It is important to have a working knowledge of copyright law, and it is helpful to have some familiarity with contracts. Publishers and authors need to read contracts and copyright transfer forms thoroughly before signing and be certain that they understand what they are agreeing to.

There are numerous Web sites containing copyright information. We recommend the following Web sites for accurate and up-to-date information, although this is by no means a complete list:

- U.S. Copyright Office, http://www.copyright.gov/
- American Chemical Society Copyright Learning Module, http://pubs.acs.org/copyright/learning_module/module.html
Obtaining Permission To Reproduce Material

Whenever an author wishes to include a figure, a table, or a substantial portion of text that has already been published elsewhere (in print or on the Internet), the author must obtain permission from the copyright holder to reproduce the material. It is the author’s responsibility to

1. identify material in a paper or manuscript that has been previously published in print or on the Internet;
2. determine whether that material is subject to copyright protection;
3. if so, identify the copyright owner and request permission in writing; and
4. ensure that permission is granted and forwarded to the author’s publisher.

The first two points are discussed at the beginning of this chapter. The second two points will be considered next in a general way applicable to requesting permission from any scientific or scholarly publisher. For information on how to reproduce materials from books, journals, or magazines published by the ACS Publications Division, see Box 7-2.

**Reminder:** Material published on an Internet site is not necessarily in the public domain, even if the site owner does not have a copyright notice on a Web page. If you download a photograph, illustration, chart, table, or text from a Web site, you must obtain permission from the copyright owner to use it in another publication. Bear in mind that the Web page publisher may not be the copyright owner.

Writing To Request Permission

Once an author has identified the tables, figures, and text that require permission, the next step is for the author to write to the copyright owner to request permission. This is not a difficult task, but it requires some organization and attention to detail, and it may take several months for permission to be granted. Fortunately, the Internet has made the task less burdensome than it used to be because most publishers post their permission policy, forms, and contact information on the Web. Some publishers now have Web-based permission systems.

**Reminder:** Bear in mind that a copyright owner is not necessarily a publisher. For example, images such as a company logo or a still shot from a movie or television commercial require permission from the corporate office or the motion picture studio or the advertising agency.

Begin by organizing your materials requiring permission according to publisher and source. This way, you can list all materials from a single publisher and source on one form, reducing paperwork for yourself and the publisher.
Determine whether the publisher has permission-request information on the Web and, if so, download or print out the appropriate request forms. (Even if the publisher has a Web-based permission system, you might want to print out the blank form, so you can be sure that you have collected the necessary information when you fill it out online.)

If the publisher does not have forms on the Web, then draft a letter requesting permission. Be sure to include the elements listed in Box 7-3.

List all the material for which you need permission from a given publisher on one form or on the form with an attachment. Unless the publisher specifically directs differently, avoid submitting one form for each item requiring permission.

Include your specific deadline date by which you wish to have the permission granted.
Box 7-3. Components of a Permission Request

Your request for permission to reproduce material will be processed more quickly by a publisher if you provide all the necessary information on the publisher’s form or in a request letter. A permission request should provide the following information:

1. A list of the original figure or table numbers for each figure or table that you wish to reproduce from a given source, along with a complete reference citation for the source.
   - The reference citation for a journal article should include the name(s) of the author(s); the name of the journal; the month, day, and year of publication; volume and issue numbers; and inclusive page numbers for the article.
   - The reference citation for a book should include the title of the book (and series name and number if applicable); the name(s) of the author(s) or editor(s); the year of publication; and the page numbers on which the original figures or tables appear. If appropriate, also list the title of the chapter, the name(s) of the chapter author(s), and the inclusive page numbers for that chapter.

2. A description of where the material will be published. Include the title of the forthcoming publication, the type of publication (e.g., journal, book, magazine, or Web journal), and the name of your publisher.

3. A list of the formats in which the requested material will appear, such as print, online, CD-ROM, or proceedings. Unless all rights are requested, only print rights will be granted.

4. Your complete mailing address, e-mail address, and telephone and fax numbers.

5. A specific deadline (calendar date).

Many permission request letters also include a space for the original publisher to specify the publisher’s preferred credit line.

Include complete contact information for yourself, including a mailing address, e-mail address, and telephone and fax numbers.

If you do not have a response from the copyright owner in a reasonable amount of time, contact the publisher again and try to determine the reasons for the delay; perhaps your request was not received or was missing information.
not assume that you have permission unless you have heard explicitly from the publisher, even if you set a deadline.

What Sort of Credit Line Is Appropriate?

Once the publisher has granted permission to reproduce materials, incorporate the required copyright credit line into your manuscript. This credit line notifies readers that the publisher owns copyright to the material. Each publisher has its own style for credit lines. For example, the credit line required by the ACS is shown below:

Reprinted with permission from REFERENCE CITATION. Copyright YEAR American Chemical Society. (Insert the appropriate information in place of the capitalized words.)

Include the credit line on the first page where copyrighted text appears and under each copyrighted table or figure.

If you are adapting or modifying copyrighted material or if parts of copyrighted material are being used, the words “Adapted” or “Reprinted in part” should replace “Reprinted” in the credit line.

Transferring Copyright

Most scientific and scholarly publishers require the transfer of copyright ownership as part of the publication agreement between the publisher and authors. When the publisher owns copyright, it removes the burden from authors to grant permission and it assures them that only legitimate requests for their material are approved. Similarly, if the publisher owns copyright, it is easier for authors who are seeking permission to come to one source that handles requests from multiple references and processes them quickly. If individual authors owned copyright, it might be difficult and cumbersome to contact authors for permission to use their works or portions of their works. If you are in doubt about a publisher’s requirements, contact the publisher or seek legal advice.

Each publisher has forms for transferring copyright to the publisher, and the submission of a completed copyright transfer form is nearly always necessary before a publisher will schedule publication of or begin production work on a manuscript. When authors publish in an ACS publication, they assign copyright interest via the ACS Copyright Status Form. This form is available on the ACS Publications Division Web site at http://pubs.acs.org/cgi-bin/display-copyright?bichaw and in the January issues of ACS journals. Authors publishing books with ACS will find a form at http://pubs.acs.org/books/forms.shtml. Completed Copyright Status Forms should be submitted to the appropriate book or journal editor, not the ACS Copyright Office.
A style guide is presumed in its basic objective as guiding authors in the task of producing a document describing their work. In a conventional sense, style is traditionally presentational in objective and is aimed at producing a (visually) homogeneous form suitable for aggregation into a journal issue or a book. At the outset of this chapter, we should pin our flag firmly to a rather different mast. This chapter is less about the application of style to the presentation of a document and more about the general principles involved in its application to data to achieve a homogeneous form capable of being reused. It is not so much about how to create a document, but rather about how to create a more data-focused entity we call a datument (1), that is, a container for data and its associated descriptions. The datument can have conventional attributes of authorship, affiliation, and other familiar structural components, such as sections, tables, figures, and bibliography, but it extends this by also carrying data. This differs from, for instance, tabulated or quoted data typical of that found in most chemical documents. To illustrate this most important difference, consider the following assertion:

The melting point of aspirin is 135°, and its molecular ion has the formula C₉H₈O₄⁺.

As a human trained in chemistry, you probably understand much of the semantics, but consider how much potential ambiguity and implied meaning is contained in this admittedly concise statement.

- You understand what is meant by the term melting point, but you might have to seek a librarian’s help to locate a relevant dictionary of chemical terms where you can check a more precise definition should the need arise.
After a little thinking, you conclude that the glyph ° indicates that the number preceding it is a temperature expressed in Celsius units. You probably also recognize that this number is probably only accurate to ± 1 °C, only because you have made such measurements yourself. At the back of your mind is probably the knowledge that a value of 135° is reasonable for an organic compound (and that 1135° would not be), that this implies that this substance is a solid at room temperature and that this value may be used as an approximate indicator of chemical purity.

You certainly recognize the term aspirin as a trivial, unsystematic but commonly used description of a nevertheless well-defined molecule (the structure, or more accurately the connection table, of which you may need to ascertain).

The term molecular ion is a term that tends to be used in a particular branch of spectroscopy known as mass spectrometry.

You have little difficulty in recognizing the molecular formula as by convention listing the number of carbon atoms as the subscript to the initial C, then followed by the number of hydrogen and then other atoms in alphabetical order. The final suffix indicates the charge on the system and reconciles with the use of the term ion, and you will notice that the suffix reveals the presence of an unpaired electron.

You probably are aware of rules that would allow you to check the validity of this formula (i.e., are the + and the · consistent with each other; is the formula physically possible within the constraints of valence theory, etc.).

You might want to derive a molecular mass from the formula, in which case you need to know about atomic weights, isotopes, and other concepts.

You might want to relate the formula to a two-dimensional structural representation, indicating perhaps where the charge might reside, or how the ion might fragment, or a three-dimensional representation for molecular modeling.

As a human, you will infer properties such as aromaticity or the probable presence of a hydrogen bond.

A knowledgeable chemist could probably make quite a few more inferences from the above, but the purpose here is to illustrate how much implicit (i.e., undeclared) information there is in such a brief statement (all well-defined chemical terms are shown above in italics to emphasize this). The purpose in writing it all down is to reinforce the idea that although such a statement (as might be found in a document) contains much data, only a human can really make significant use of it. Well, that would be true only if the human were to give undivided attention to the contents of such a document; the human certainly could not cope well with more than a few such documents, and not at all with, say, millions of documents. A normal response to such issues of scale would be to say that the essential data and semantics of the above phrase need to be abstracted (with inevitable loss
of some data and information) into a database representation and then suitably queried if needed; after all, agencies such as Chemical Abstracts Service exist to provide such a service. However, consider that the process of converting even a brief statement such as the above into a true chemical abstract requires an expert (and it must be said, error-prone) human. Even then, the knowledge required to construct the list above would have to be acquired from other sources.

Could instead much, perhaps all, of this work be handled by a computer? The answer is a clear “yes”, but only if the ground is well prepared for such a task. The purpose of this chapter is to outline some of the basic principles (but not the technical details) of how this could be done and to set out the grander vision that creating an infrastructure that adopts such principles would be the first step toward what has been described as a semantic web of information and knowledge. Not only humans but machines could roam, on vast scales if need be, on such a web, and by doing so discover connections between data and concepts which in days past might have been described as the art of scientific serendipity.

### Markup Languages and the World Wide Web

The World Wide Web arose from the need for high-energy physicists at Conseil Européen pour la Recherche Nucléaire (CERN) to communicate and exchange data and information within a large dispersed community. The basic design, which has been well documented, involved the creation of structured documents containing identifiable information components linked by uniform resource identifiers using markup tags that could be recognized by machines and used as formatting or styling instructions rather than being part of the actual content. Using the HTML version of the previous example:

```html
<p>The melting point of aspirin is 135°; and its molecular ion has the formula C<sub>9</sub>H<sub>8</sub>O<sub>4</sub>+. </p>
```

The “tags” in the angle brackets are recognized by the processor as markup and are used as instructions rather than content to produce the previously rendered sentence. Although such examples will be familiar to many readers, we emphasize it here because it illustrates the critical importance of separating content from style (or form). The `<p>` tags precisely define a paragraph, a unit for structuring the document. A machine could now easily count the paragraphs in a document and the number of characters (but not individual words, which are separated not by tags, but by spaces) in each. HTML provides a flexible (perhaps rather too flexible) document structure for text (paragraphs, headers, tables, lists), embedded images (and other multimedia objects), human interactivity (through forms), programs (through scripts, applets, and plug-ins), styling (some degree of formatting and screen layout), and metadata (essentially descriptions of data).
Whereas this is a substantial list, its success has generated many problems, which HTML in its original form cannot solve:

- HTML can only support a fixed tagset (for example 59 in the latest specification for XHTML 2.0), and even this number is regarded as close to unmanageable (no software yet implements this full set consistently, accurately, and completely). Any other tags that might be present (e.g., `<molecule>`) are simply ignored (strictly speaking, they should be marked as invalid HTML, although they may be valid for other languages).
- Much of the behavior (semantics) is undefined. This lack has led to specific disciplines creating their proprietary methods of supporting functionality (e.g., through scripting languages, plug-ins, applets, and other software).
- HTML was designed to be error-tolerant, in recognition that it would be authored (and viewed) mostly by humans. Browsers may try to recover from nonconforming documents and may do so in different ways. Humans are good at recognizing and often correcting errors in HTML (missing links, broken formatting, incomplete text). Machines cannot normally manage broken HTML other than in a “fuzzy” manner.
- Author-provided metadata is often entirely absent. If present, it will likely adhere to a general form (the so-called Dublin Core schema, http://dublincore.org/), of limited utility in scientific, technical, and medical (STM) areas.
- The emphasis on presentation in many of the original tags (such as fonts, colors, and layout) muddled the separation of content from style. The World Wide Web Consortium soon developed technologies (CSS, or cascading style sheets, and XSL, or extensible stylesheet language; more information on this and other XML issues is available at http://www.w3c.org/) to help overcome this problem, but as with HTML, CSS is variably implemented in most browsers. Most commercial tools for authoring HTML emphasize presentation or interactivity (to capture the reader’s attention), and in such HTML, the content is subservient to the style.

*Examples of XML and of Chemical Markup Language*

These conventional markup approaches (HTML, CSS, and XSL) are inadequate for dataments because there is usually no domain-specific support. XML, or extensible markup language, was introduced as a solution to this problem. XML was designed to be simple, easy to use, and small; it is a fully conforming subset of the older SGML (essentially “SGML lite”). It allows new markup languages to be defined through an XML schema formalism (see http://www.w3c.org/XML/Schema). A schema specifies a set of rules (syntax, structure, and vocabulary) to which a document must conform; those that do are said to be “valid”. Schemas allow more precise constraints, allow the definition of datatypes, and enhance the potential for machine processing.
We start by explaining the terms used in the XML language, illustrated with a small and simple example (kept brief for simplicity and hence not relating to a real molecule) (Scheme 8-1).

```
<molecule>
  <identifier convention="CAS-RN">150-78-2</identifier>
  <identifier version="1.0" convention="InChI">1.0/C9H8O4/c1-6(10)13-8-5-3-2-4-7(8)9(11)12/...</identifier>
  <atomArray>
    <atom id="a1" elementType="C" x2="-5.4753" y2="5.0867"/>
    <atom id="a2" elementType="C" x2="-5.4753" y2="3.5466"/>
  </atomArray>
  <bondArray>
    <bond atomRefs2="a1 a2" order="2"/>
  </bondArray>
</molecule>
```

Scheme 8-1. The basic features of an XML document.

The core of the language consists of a set of data containers, or more formally elements (not to be confused with the chemical elements), the enumeration of which is ideally defined by a schema. In this example, the elements are `<molecule>`, `<identifier>`, `<atomArray>`, `<atom>`, `<bondArray>`, and `<bond>`. These have a clearly defined relationship to one another (illustrated above by indentation of the text). Thus the element `<atomArray>` is said to be the parent of a child element termed `<atom>`, and both are children of the top-level element `<molecule>`, which can also be called the document root element. This hierarchy among elements is precisely defined and must carry no ambiguity.

Elements can specify data or information in two ways. First, data can be contained between the start and end of any particular element, such as `<identifier>` and `</identifier>` in the example. Such content can of course be other (child) elements, but it can also be character or numeric data, as in the example above, which uses both the CAS Registry Number, a unique identifier assigned to chemical structures by CAS (see Appendix 12-3), and a unique canonical molecule identifier known as InChI (International Chemical Identifier) (for more on InChI, see Appendix 8-1).

Second, data can also occur as the value of an attribute to the element. In the example above, the `<identifier>` element has two attributes, `version="1.0"` and `convention="InChI"`. Both the name of the attribute and its value can be enumerated if needed by the schema; if the attribute is unknown, or its value is outside defined limits, the entire document or datument can be flagged as invalid by suitable software. Thus `<atom>` has attributes `elementType="C"` and `x2="-5.4753"`. For the former, a value of “C” is allowed (because it is recognized as the standard symbol for the chemical element carbon), but a value of say “CX” would not be allowed. The second attribute is defined (in the schema) as the x coordinate of a set of two-dimensional molecular coordinates. As such, its presence implies that it should be paired with a y2 coordinate. One can specify in the
schema what kind of behavior to impose if, say, $y_2$ were to be missing. One might decide that its presence would be inferred and that its value should be $y_2=0.0$, although in practice that would be a dangerous assumption, and it would be better to flag its absence as an error. Decisions also have to be made regarding the value of this attribute. With two-dimensional coordinates, no assumptions can really be made about the units in which the coordinates are specified, and it would be up to any software to process the values in a sensible manner. Whereas a human might think that, e.g., $x_2=-54753.0$ looks unreasonable, it may still be internally consistent with the other coordinates. Such software would probably also be expected to trap conditions such as two atoms with identical coordinates, or truly unreasonable values. However, one can be a little more specific about, e.g., $x_3=-5.4753$. This would be interpreted as the $x$ coordinate of a three-dimensional set, and as such a reasonable implicit behavior would be to treat this value as corresponding to Angstrom units unless otherwise specified. It is also worth noting that elements which specify data in the form of attributes need not enclose any further data; thus `<atom/>` in this case represents both the start and the end of the element (in other words it is an empty container).

The preceding discussion has been fairly precise and meticulous, if only to illustrate how XML can be used to impose well-defined structures and relationships on data. We emphasize, however, that it would not normally be a human who has to cope with such levels of detail and precision; the design is such that in fact software will carry almost all of the burden of producing the XML in the first place and then validating and using it subsequently. The preceding argument served only to illustrate how such software can be made to safely operate without the need for human intervention in the process.

The second example (Scheme 8-2) is an elaboration of the first fragment, but formalized below as CML (chemical markup language) (3). We emphasize that this chapter is not meant to be an instructional manual for any given markup language, with CML here serving only to illustrate the general principles involved. Many other scientific applications of XML have been developed (3, 4), and syntactically, either of these examples could be replaced by other such modularized markup languages.

This more extensive example illustrates how a wider range of properties can be defined and also contains a new feature called a namespace. The purpose of this namespace is to enable this entire XML fragment to be combined or aggregated with other XML languages so that no conflict between the names used for the elements can arise. This aggregation is achieved by prefacing each element with a unique (to the document) short string: `<cml:molecule>`. An attribute `xmlns:cml` is now used to define what is called a URI (uniform resource identifier), which stamps a globally unique identifier on the meaning of the `cml:` prefix. This uniqueness will allow this datum to coexist with other XML languages without conflict (an example of which is described later in this chapter).
Scheme 8-2. A CML datumment describing a property of aspirin.

The molecule element in this example contains five child elements: cml:metadata, cml:identifier, cml:atomArray, cml:bondArray, and cml:propertyList. Of these, cml:metadata, cml:atomArray, and cml:bondArray have no children and are empty containers, defining only attribute/value pairs, whereas cml:propertyList has one child, cml:property. The latter itself has a child: cml:scalar. As well as the namespace, the cml:molecule element itself has two other attributes, id and title.

The </cml:property> and </cml:scalar> elements reference namespaces other than CML. This is done to facilitate aggregation with other XML components, such as dictionaries, and by this means to reduce what has been called “tag soup”. For example, <cml:property dictRef="chem:mpt"/> defines a namespace for a dictionary reference called chem:mpt. Any processing software that might need to process a melting point property would be directed to this dictionary for further information on the semantics of this term. Similarly, the
attribute `units=“unit:c”` would handle the conversion of scientific units, and `dataType=“xsd:decimal”` would handle the basic datatype (i.e., the definition of a decimal number) itself. This mechanism avoids overburdening CML itself with the need to specify such semantics. No other elements or attributes in this example have XML-defined semantics; all other semantics are imposed by CML itself. Thus, the CML schema defines an enumeration (list) of allowed `elementType`s and defines their meaning, use, and boundaries. These aspects are discussed in more detail below.

**The Use of Identifiers**

The examples of XML shown in Schemes 8-1 and 8-2 illustrate the use of two types of identifiers. The identifier attributes seen in, e.g., `<cml:atomArray atomID="a1 a2 a3 a4 a5 ...">` are used internally to enable specification of, e.g., `<cml:bondArray atomRef1="a5 a1 a2 ...” atomRef2="a1 a2 a3 ...“>` and should be unique within the datument (but not necessarily globally) to ensure that this XML document is well-formed and valid. The second type is an element containing identifiers. Various identifiers could be used, such as SMILES, CAS-RN, and the InChI canonical identifier (as shown here), precisely derived from the molecule connection table and used to establish molecular global uniqueness. Any two datuments that contain the same InChI identifier (in this example, `C9H8O4/c1-6(10)13-8-5-3-2-4-7(8)9(11)12/h1H3,2-5H,(H,11,12)` should be presumed to refer to the same molecule (in the sense of a connection table, but not necessarily other properties, such as 3-D coordinates, for example). The whole aspect of identifiable data is pivotal to the concepts used here. The CAS-RN is widely used and offers comprehensive coverage from simple molecules to polymers to Markush structures. The InChI can be derived from the structure, but it is still a fairly new standard. It does not yet have wide support and does not yet offer complete coverage of all materials.

**Display of XML and Specific XML Languages**

The default way of “displaying” or “browsing” any XML-compliant language, such as CML, is as a so-called tree view, outlining the structure of the document (Figure 8-1) but to which no style has been applied. Most modern Web browsers will support this feature (we recommend Firefox).

Of more utility is to associate a specific style or transform with this datument. A technology known as XSLT is essentially a specification of how an XML-based datument might be transformed into a different representation (or subset) of the data. Four examples of how this might be used to transform this datument are listed below:

- Extraction of atom two- or three-dimensional coordinates and rewrapping with appropriate syntax for interactive display on screen using appropriate
Chapter 8: Markup Languages and the Datument

(A)  
```xml
<cml:molecule id="m01" title="aspirin">  
    <cml:atomArray atomID="a1 a2 a3 a4 a5 a6 a7 a8 a9 a10 a11 a12 a13"  
      elementType="C C C C C C C O O O O" formalCharge="0 0 0 0 0 0 0 0 0 0 0 0"  
      hydrogenCount="1 1 1 0 0 0 0 3 0 1 0 0"  
      x2="-5.475336 -5.475336 -4.141667 -2.807998 -4.141667 -4.141667  
          -2.807988 -1.075737 -1.075737 -5.629193 -2.807988 -1.474318  
          0.464263"  
      y2="5.086684 3.546650 2.776633 3.546650 5.856650 5.856650  
          7.396700 5.086684 7.344209 8.884209 7.795282 8.166700 5.856684  
          7.344209"  
    >  
    <cml:bondArray atomRef1="a5 a1 a2 a3 a4 a5 a6 a7 a12 a8 a8"  
      atomRef2="a1 a2 a3 a4 a7 a6 a11 a10 a12 a8 a13 a9"  
      order="1 2 1 2 1 1 2 1 1 2 1"  
      order="1 2 1 2 1 1 2 1 1 2 1"  
      order="1 2 1 2 1 1 2 1 1 2 1"  
      order="1 2 1 2 1 1 2 1 1 2 1" />  
</cml:molecule>
```

(B)  
```xml
<cml:molecule id="m01" title="aspirin">  
    <cml:metadata name="dc:identifier" content="InChI"/>  
    + <cml:identifier version="1.0" convention="InChI"></cml:identifier>  
    <cml:metadata name="dc:identifier" content="CAS-RN"/>  
    <cml:identifier convention="CAS-RN">150-78-2</cml:identifier>  
    <cml:atomArray atomID="a1 a2 a3 a4 a5 a6 a7 a8 a9 a10 a11 a12 a13"  
      elementType="C C C C C C C O O O O" formalCharge="0 0 0 0 0 0 0 0 0 0 0 0"  
      hydrogenCount="1 1 1 0 0 0 0 3 0 1 0 0"  
      x2="-5.475336 -5.475336 -4.141667 -2.807998 -4.141667 -4.141667  
          -2.807988 -1.075737 -1.075737 -5.629193 -2.807988 -1.474318  
          0.464263"  
      y2="5.086684 3.546650 2.776633 3.546650 5.856650 5.856650  
          7.396700 5.086684 7.344209 8.884209 7.795282 8.166700 5.856684  
          7.344209"  
    >  
    <cml:bondArray atomRef1="a5 a1 a2 a3 a4 a5 a6 a7 a12 a8 a8"  
      atomRef2="a1 a2 a3 a4 a7 a6 a11 a10 a12 a8 a13 a9"  
      order="1 2 1 2 1 1 2 1 1 2 1"  
      order="1 2 1 2 1 1 2 1 1 2 1"  
      order="1 2 1 2 1 1 2 1 1 2 1"  
      order="1 2 1 2 1 1 2 1 1 2 1" />  
</cml:molecule>
```

(C)  
```xml
<cml:molecule id="m01" title="aspirin">  
    <cml:metadata name="dc:identifier" content="InChI"/>  
    + <cml:identifier version="1.0" convention="InChI">1.0/c9h8O4/c1-6(10)13-8-5-3-2-4-7(8)9(11)12/h1H3, 2-5H, (H,11,12)</cml:identifier>  
    <cml:metadata name="dc:identifier" content="CAS-RN"/>  
    <cml:identifier convention="CAS-RN">150-78-2</cml:identifier>  
    <cml:atomArray atomID="a1 a2 a3 a4 a5 a6 a7 a8 a9 a10 a11 a12 a13"  
      elementType="C C C C C C C O O O O" formalCharge="0 0 0 0 0 0 0 0 0 0 0 0"  
      hydrogenCount="1 1 1 0 0 0 0 3 0 1 0 0"  
      x2="-5.475336 -5.475336 -4.141667 -2.807998 -4.141667 -4.141667  
          -2.807988 -1.075737 -1.075737 -5.629193 -2.807988 -1.474318  
          0.464263"  
      y2="5.086684 3.546650 2.776633 3.546650 5.856650 5.856650  
          7.396700 5.086684 7.344209 8.884209 7.795282 8.166700 5.856684  
          7.344209"  
    >  
    <cml:bondArray atomRef1="a5 a1 a2 a3 a4 a5 a6 a7 a12 a8 a8"  
      atomRef2="a1 a2 a3 a4 a7 a6 a11 a10 a12 a8 a13 a9"  
      order="1 2 1 2 1 1 2 1 1 2 1"  
      order="1 2 1 2 1 1 2 1 1 2 1"  
      order="1 2 1 2 1 1 2 1 1 2 1"  
      order="1 2 1 2 1 1 2 1 1 2 1" />  
</cml:molecule>
```

Figure 8-1. Viewing the XML datument described in Scheme 8-2 in a Web browser, shown as (A) a collapsed tree view, (B) partially expanded, and (C) fully expanded.
software. This use was first demonstrated in an unusual series of articles about themselves, in which the theme was to demonstrate how they could be dynamically transformed into other representations of the data contained within (5–7).

- Use of the atom array to calculate a molecular formula and weight.
- Calculation of molecular properties via invocation of molecular modeling algorithms using, e.g., Web services.
- Use as a database query (“Is aspirin in this database?”).

Only the first of these uses really corresponds to the conventional sense of a document (whether it be an HTML page on the Web or a journal article in PDF format). The last three uses would be true applications of the datument as part of a semantic web. Another difference is that the semantics in such a datument cannot be unambiguously deduced from inspecting such examples but must be formally defined (e.g., in an XML schema or similar tool). Thus, CML2 defines that, e.g., the \texttt{atom\_Ref1} and \texttt{atom\_Ref2} attributes (of the element \texttt{bond\_Array}) contains references to \texttt{id} attributes on \texttt{atom\_Array} elements and that the \texttt{order="1"} attribute relates to a single bond. How a single bond is handled must in turn be specified by the software; a display program may render the bond in a particular width, color, taper, etc., whereas a database query may handle this information quite differently, or indeed not need it at all.

**Datument Validation**

Publishers often provide human-readable guidelines for authors (also known as style guides) for document preparation, which sometimes can extend to entire books. Humans are also quite prone to noncompliance or imperfect compliance because they are often busy or perhaps simply readily bored. Guidelines for data preparation, if they exist, are often to be found in optional categories, such as supporting information. If an author deposits data in such a form, how does the publisher know that it is correct? A key aspect of XML is that documents (and of course datuments) can be validated. For publishing purposes, validation implies a contract between the author and the publisher, which is machine-enforceable. A schema formalizes the syntax, vocabulary, document structure, and some of the semantics. It comprises a set of machine-based rules to which a datument must conform. If it does not, it is the author’s responsibility to edit it until it does. If it conforms, it is assumed that the author has complied with the publisher’s requirements.

Validation guarantees that the datument conforms to rules. The more powerful the rules, the more invalid data can be detected. Thus, schemas can allow the detection of some disallowed data, particularly with a controlled vocabulary. An atom in CML is not allowed an \texttt{elementType} of “CO” (arising perhaps as a mis-
print for the element “Co”), or a hydrogenCount of –1. It is, however, allowed a formalCharge of “+10”. This might be corrupted data or a legitimate description of a highly ionized atom. Individual schema-based rules (e.g., for different journals) could allow discrimination between these possibilities.

**Datument Vocabularies**

The construction of a schema immediately emphasizes the need for a communal vocabulary. An element such as `<molecule>` must be processed in the same consistent manner regardless of the author, the reader, or the processing software. We emphasize “processing”; the implementor must adhere to the same software specifications, and the software must behave in a predictable manner. For many scientists, this implementation will require a change in their thinking, and we emphasize the consequences here.

In its strictest form, this attitude is a controlled vocabulary. Only certain terms may be used, and their meaning is specified by a trusted authority. An example is IUPAC “gold book” vocabulary of chemical terms and definitions (at http://www.chemsoc.org/chembytes/goldbook/). Controlled vocabularies are widely used to enforce the mapping of a discipline such as chemistry onto a generally agreed or mandated vocabulary. They often require substantial formal guidelines or training sessions to ensure consistency of interpretation. Markup languages require us to use absolute precision in syntax and structure. It is highly desirable to have additional precision in semantics (the meaning and behavior of documents). The attachment of semantics to documents is not generally appreciated but is a critical process, and we must have a formal means of attaching semantics to every XML element and attribute and their content. At present, this can be achieved in four principal ways, ordered below in terms of machine-understandable rigor.

**A Human-Readable Prose Description**

This description can be as simple as a definition in a dictionary, which may or may not give an indication as to how it might be used. An example from the CIF (crystallographic) dictionary is `_chemical_compound_source`, which is defined as “description of the source of the compound under study, or of the parent molecule if a simple derivative is studied. This includes the place of discovery for minerals or the actual source of a natural product.” This description formalizes the concept but (deliberately) gives wide latitude in its implementation and content.

**A Human-Readable Set of Instructions for Machine Implementation**

Another CIF entry (abbreviated) for `_atom_site_U_iso_or_equiv` might specify carefully how the concept must be implemented and indicate constraints, such as datatype, enumeration range, and units. The constraints are all machine-processable, and the definition includes an implementable algorithmic constraint.
Because CIF predates XML, this definition is not machine-processable (i.e., it acts as a specification for a human programmer, but it cannot be used to generate software automatically). XML schemas provide mechanisms to overcome this.

**Definitions by Software**

Many elements of a controlled vocabulary are effectively defined by software implementation. Thus, the description of the HTML language requires certain elements to have specified behavior. For example, `<img>` supports the display of raster images, but the precise look may vary between implementations and file types. Implementation through software is useful and powerful where authors, publishers, readers, and processors all use the same system. Because STM publishing is increasingly multidisciplinary, this implementation becomes problematic. Often a reader may have to download specialist software that is idiosyncratic and that may not have enough functionality, especially the export of semantically rich data. Moreover, the semantic rules are often buried deep in the software and difficult to understand precisely.

**Formal Semantics**

We believe that the chemical community should move toward the adoption of formal rules for expressing semantics and ontology (semantics is the branch of semiotics, the philosophy or study of signs, that deals with meaning. Ontology is defined as a description, such as a formal specification of a program, of the concepts and relationships that can exist for an agent or a community of agents). Our central message is that we need carefully constructed and curated machine-processable ontologies. We believe that scientific and scholarly organizations have a major role to play and that openness and free access to ontologies is critical.

**Authoring and Editing Tools**

At present, most chemical publications are created by authors in a publisher-specific manner. Each publisher requires a particular document structure, often a particular technology (e.g., formats of text, images, references, and domain-specific data) and a particular (usually implicit) ontology. The author has to change each of these according to the publisher’s requirements and independently of the content. The publisher (or author) then has to make significant technical edits, often as a result of author noncompliance. Original data are transformed into text-oriented formatting languages for rendering to human-readable output, either paper or e-paper, and during this process the machine-processability is lost. Supporting data are often prepared in a variety of (ill-suited) formats; thus, spectral information is frequently merely a scanned image corresponding to the original printed spectrum (itself formatted for human convenience rather than processability).
XML has the potential to revolutionize this situation. With agreed XML-based markup languages, authors can have a single environment independent of the publishers’ requirements. Publishers can transform the XML into their in-house systems, but quite independently other “reusers” can do so to their own (possibly quite different) requirements. The original datument, which contains all the “supporting data”, can be archived along with the semantics and ontology, all in XML. To achieve all of this consistency, a major change will be required in authoring tools. Instead of proprietary text-based tools, with little useful support for semantics of either text or data, we will require XML-based tools with domain-specific XML components.

An XML editor display environment contains generic mechanisms to manage any domain-specific schema and therefore ensures that a resulting datument is valid. It will also contain mechanisms for supporting domain-specific software, such as editors and browsers (e.g., for molecules, spectra, etc.). Much high-quality chemistry software capable of being used in this context is already available. One commercial example based on XML, which encapsulates this concept, has already appeared. The Publicon tool, for example, provides a comprehensive technical authoring environment capable of handling mathematics and expressing the result in XML; interestingly, its target audience includes chemists and bioscientists. Because all XML-conforming markup languages have essentially the same kinds of structures, syntax, and rules, it becomes much easier to write appropriate, often generic, software to handle it.

**The Datument as a Component of a Scientific Grid**

The use of XML has the potential to create savings in certain areas (time for authors and staff costs for technical editors), but a major benefit is that the collected XML datuments, together with the ontologies, would effectively create a machine-processable knowledge base for chemistry. At present, primary publications do not create knowledge without a lot of additional human actions to maximize the knowledge created by primary publications: abstracting, collating, and validating are needed. If this knowledge could be captured and tagged within the primary publication itself, without simply transferring that human action to a different point in the process, a significant proportion of the knowledge base could be extracted by machine. If the metadata, structure, datatypes, ontology, semantics, and processing behavior of a piece of information are determined, it essentially becomes a self-describing *information component*. These information components—which might be implemented by a mixture of XML protocols and object-oriented code—can be regarded as stand-alone, self-describing parts of a knowledge base. Protocols such as XML Query are able to search a heterogeneous aggregate of such components, and RDF (resource description framework, a way
to use metadata so that, for example, search engines can locate it) will be able to make deductions from their metadata. By combination of different markup languages, all information, even at a fine level, can be captured without loss. Any part of it can be retrieved, and hence a collection of marked up XML publications would constitute a knowledge base.

If each datument has sufficient high-quality metadata, there may be no essential need for a knowledge base to be centralized. By collecting those publications of interest, any reader or group can create their own personal base. In turn, such metadata can be exported to a wider community using new mechanisms such as RDF or RSS (RDF Site Summary or Rich Site Summary, a way of collecting metadata of interest to an individual reader).

With such exciting technologies in the offing, authors, funders, editors, publishers, and readers have a unique opportunity to start experimenting with creation and dissemination of machine-understandable information and data as an integral part of the process of scientific publishing.

References

4. A full review and listing of all scientifically based XML languages is beyond the scope of this short chapter. Other than CML, the best documented is ThermoML, which is used for thermophysical and thermochemical data. Frenkel, M.; Chirico, R. D.; Diky, V. V.; Marsh, K. N.; Dymond, J. H.; Wakeham, W. A. *J. Chem. Eng. Data* 2004, 49, 381–393 and references cited therein.
The ability to represent uniquely a chemical compound is a fundamental requirement for storage or transmission of chemical information. We define compounds by their molecular structure, as shown in two-dimensional diagrams or stored in computers. Pronounceable names have been developed for oral and written communication, ranging from the trivial, containing no structural information, to completely systematic names, which can be decoded to yield the original structure. However, the application of systematic nomenclature to complicated structures requires expert knowledge of elaborate systems of nomenclature rules. The use of systematic nomenclature to convey information about the increasingly complex molecular systems handled by today's chemists is both laborious and inefficient.

Over the past decade, with ever-increasing reliance by chemists on computer processing, the International Union of Pure and Applied Chemistry (IUPAC) recognized a need to develop methods of nomenclature that can be interpreted by computers, or more precisely, by computer algorithms. A new program was initiated, aimed at creating a method to generate a freely available, nonproprietary identifier for chemical substances that could be used in printed and electronic data sources. The technical development was carried out primarily at the U.S. National Institute of Standards and Technology, and the product is referred to as the IUPAC International Chemical Identifier (InChI).

InChI is not a registry system. It does not depend on the existence of a database of unique substance records to establish the next available sequence number for any new chemical substance being assigned an identifier. Instead, InChI transforms the chemical structure of a compound into a string of characters that uniquely identify that compound. This conversion of a graphical representation of a chemical substance into the unique InChI label can be carried out automatically by any organization, and the facility can be built into any chemical structure drawing program. InChI labels are completely transferable and can be created from existing collections of chemical structures.

Whereas the theory needed for conversion of a structure to a unique string of characters has been known for a long time, when work on InChI began there were no freely available unique representations for compound identification, nor
was their development being actively discussed. Thus, before active development could proceed, a precise specification of requirements was wanted, and the following five characteristics were specified as needed for such an identifier:

1. The structure of the compound can be drawn using common conventions.
2. The identifier is derived directly from the structure by an algorithm.
3. Exactly one identifier is associated with a given structure, that is, different structures give different identifiers.
4. The identifier works for a large fraction of all “drawable” chemical substances.
5. The identifier must be openly available.

To be as precise and broadly applicable as desired, InChI uses a layered format to represent all available structural information relevant to compound identity. Each layer in an InChI representation contains a specific type of structural information. These layers, automatically extracted from the input structure, are designed so that each successive layer adds additional detail. The specific layers generated depend on the level of structural detail available and whether tautomerism is allowed. Any ambiguities or uncertainties in the original structure will remain in the InChI. The InChI layers are formula (standard Hill sorted); connectivity (no formal bond orders), including disconnected and connected metals; isotopes; stereochemistry, including double bond (Z/E) and tetrahedral (sp³); and tautomers (on or off). Charges are not part of the basic InChI, but rather are added at the end of the InChI string.

An example of an InChI representation is given in Figure 8A-1. The acronym InChI and version number are regarded as part of the InChI string (InChI=1 in this case). It is important to recognize, however, that InChI strings are intended for use by computers, and end users need not understand any of their details. In fact, the open nature of InChI and its flexibility of representation, after implementation into software systems, may allow chemists to be even less concerned with the details of structure representation by computers. Source code and an executable version of the structure-to-InChI conversion algorithm are freely available from the IUPAC InChI Web site at http://www.iupac.org/inchi.

InChI=1/C5H5N5O/c6-5-9-3-2(4(11)10-5)7-1-8-3/h1H,(H4,6,7,8,9,10,11)/f/h8,10H,6H2

Figure 8A-1. InChI for guanine: (A) input structure; (B) mobile H canonical numbering, with the attachment points of four mobile H and changeable bonds indicated in bold; and (C) with fixed H canonical numbering.
This chapter presents grammatical points that cover most situations. It does not attempt to discuss all the rules of grammar; many excellent grammar texts are available for that purpose, such as those given in the selected bibliography, Chapter 18. Writing style and word usage are discussed in Chapter 4. Punctuation, spelling, and word usage are also discussed in Chapter 11 with respect to numbers, mathematics, and units of measure and in Chapter 12 with respect to chemical names.

Grammar

Subject–Verb Agreement

Everyone knows that a subject and its verb must agree in number. Nevertheless, errors in subject–verb agreement are quite common. The primary cause is confusion about the number of the subject.

➤ The number of the subject can be obscured when one or more prepositional phrases come between the subject and the verb.

Application of this technique to studies on the phytoplankton biomass and its environments is described. (The subject is “application”, which is singular.)

➤ The number of the subject can be obscured when the sentence is constructed in the order prepositional phrase, verb, subject.

To the mixture were added KCl, HEPES, and water.

To the solution was added the parent compound.
The ACS Style Guide

Two singular subjects joined by “and” require a plural verb.

Growth and isolation of M13 virus were described.

**EXAMPLE** A subject that is plural in form but singular in effect takes a singular verb. Here a compound subject functions as a single entity.

Research and development is attracting a growing number of young scientists.

Its inventor and chief practitioner is a native son of Boston, Robert Coles.

Much inconsistency and confusion exists with technical documentation.

When two or more subjects are joined by “or”, the verb takes the number of the closer or closest subject.

All of the pH values or the median pH value was used.

The median pH value or all of the pH values were used.

Collective nouns take a singular verb when the group as a whole is meant; in that case, they are often preceded by the word “the”. Collective nouns take a plural verb when individuals of the group are meant; in that case, they are often preceded by the word “a”.

<table>
<thead>
<tr>
<th>contents</th>
<th>majority</th>
<th>range</th>
</tr>
</thead>
<tbody>
<tr>
<td>couple</td>
<td>number</td>
<td>series</td>
</tr>
<tr>
<td>dozen</td>
<td>pair</td>
<td>variety</td>
</tr>
<tr>
<td>group</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The number of metal amides synthesized was the largest to date. (Refers to the number as a unit.)

A number of metal amides were synthesized. (Refers to each amide.)

The series of compounds was prepared to test the hypothesis. (Refers to the series as a unit.)

A series of compounds were tested. (Refers to each compound.)

The variety of materials tested was sufficient for comparative analysis. (Refers to variety as a unit.)

A variety of materials were tested for selective removal of $^{90}$Sr from nuclear waste solutions. (Refers to the materials individually.)

This group of workers is well aware of its responsibilities. (Refers to the group as a unit.)

This group of workers are willing to sign their names. (Refers to the individuals.)

“Data” can be a singular or plural noun.

After the data is printed and distributed, we can meet to discuss it. (Refers to the whole collection of data as one unit.)

Experimental data that we obtained are compared with previously reported results. (Refers to the data as individual results.)
Units of measure are treated as collective nouns that take a singular verb.

The mixture was stirred, and 5 mL of diluent was added.

Five grams of NaCl was added to the solution.

Three weeks is needed to complete the experiment.

To the mixture was added 5 g of compound B.

Under high pressure, 5 volumes of solution A was added.

Nouns ending in “ics” and denoting a scientific discipline are usually singular.

- dynamics
- mechanics
- kinetics
- physics
- mathematics
- thermodynamics

Mechanics involves the application of Newton’s three laws of motion.

The kinetics of electron transfer to and from photogenerated radicals was examined by laser flash photolysis.

The thermodynamics is governed by the positions of the valence and conduction bands.

Compound subjects containing the words “each”, “every”, and “everybody” take singular verbs.

- Each flask and each holder was sterilized before use.
- Every rat injected and every rat dosed orally was included.
- Everybody in the group and every visitor is assigned a different journal each month.

Sometimes, one of these words is implicit; such cases take a singular verb.

- Each name and address is entered into the database.

If both components of the compound subject do not contain, explicitly or implicitly, one of the words “each”, “every”, or “everybody”, the verb must be plural.

- Each student and all the professors were invited.

Indefinite pronouns themselves (or adjectives combined with the indefinite pronoun “one”) can be the subject of the sentence.

- Those that take a singular verb are “each”, “either”, “neither”, “no one”, “every one”, “anyone”, “someone”, “everyone”, “anybody”, “somebody”, and “everybody”.

- Each was evaluated for its effect on metabolism.
- Neither disrupts the cell membrane.
Regarding compounds 1–10, every one reacts with the control agent.
Someone measures the volume every day.

• Those that take a plural verb are “several”, “few”, “both”, and “many”.
Several were evaluated for their effects on metabolism.
Few disrupt the cell membrane.
Regarding compounds 1 and 2, both react with the control agent.
Many were chosen to be part of the study.

• Those that take either a singular or a plural verb, depending on context, are “some”, “any”, “none”, “all”, and “most”. The number of the object of the preposition determines the number of the indefinite pronoun related to it.
All of the money was stolen.
Most of the books were lost.
Not all the disks are here; some were lost.

➤ When a fraction is the subject of the sentence, the number of the attendant object of the preposition determines the number of the subject.

One-third of the precipitate was dissolved.
One-fourth of the electrons were excited.

➤ When a subject and its predicate noun disagree in number, the verb takes the number of the subject. (A predicate noun is the “complement” of a form of the verb “to be”; it refers to the same person or thing as the subject.)

The preparation and structure determination [plural subject] of these three compounds are the topic [singular predicate noun] of this paper.
The topic of this paper [singular subject] is the preparation and structure determination [plural predicate noun] of these three compounds.

Awkward Omissions of Verbs and Auxiliary Verbs

➤ Each subject in a compound sentence must have the proper verb and auxiliary verb.

INCORRECT
The eluant was added to the column, and the samples collected in 10 mL increments.

CORRECT
The eluant was added to the column, and the samples were collected in 10 mL increments.
Restrictive and Nonrestrictive Expressions

A phrase or clause is restrictive when it is necessary to the sense of the sentence; that is, the sentence would become pointless without the phrase or clause. Restrictive clauses are best introduced by “that”, not “which”.

It was necessary to find a blocking group that would react with the amino group but not with the hydroxyl group.

Comparison will be restricted to acetylene compounds that have the same functional end groups.

If the clauses beginning with “that” were deleted, the sentences would not convey the information intended. Therefore, the clauses are restrictive.

Phrases can also be restrictive.

Reactions leading to the desired products are shown in Scheme 1.

If the phrase “leading to the desired products” were deleted, the sentence would not convey the information intended.

A phrase or clause is nonrestrictive if it adds information but is not essential; that is, the sentence does not lose its meaning if the phrase or clause is deleted. Nonrestrictive phrases and clauses are set off by commas. Nonrestrictive clauses may be introduced by “who” or “which” but not by “that”.

Squalene, a precursor of cholesterol, is a 30-carbon isoprenoid.

This highly readable book, written in nontechnical language, surveys the field of chemistry by describing the contributions of chemistry to everyday life.

Moore, working at the Rockefeller Institute, developed methods for the quantitative determination of amino acids.

The current–voltage curves, which are shown in Figure 6, clearly demonstrate the reversibility of all four processes.

Several hazardous waste disposal sites are located along the shores of the Niagara River, which is a major water source.

Melvin Calvin, who won the Nobel Prize in 1961, elucidated the biochemical pathways in photosynthesis.

James Aberdeen, professor emeritus of Central State University, which has provided significant scholarship support to minority students over the years, made a generous contribution to the school’s building fund.

Dangling Modifiers

A dangling modifier is a modifying word or phrase that does not clearly and logically modify another word in the sentence. In scientific writing, the passive voice is often necessary (“the solutions were heated”; “melting points were determined”), but its use can lead to dangling modifiers.
If a modifier precedes the subject of a sentence, it must modify that subject and be separated from it by a comma. Otherwise, it is a dangling modifier.

**INCORRECT**
Splitting the atom, many new elements were discovered by Seaborg.

**CORRECT**
Splitting the atom, Seaborg discovered many new elements.

**INCORRECT**
Upon splitting the atom, many new elements were discovered by Seaborg.

**CORRECT**
Upon splitting the atom, Seaborg discovered many new elements.

**INCORRECT**
When confronted with these limitations, the experiments were discontinued.

**CORRECT**
When confronted with these limitations, we discontinued the experiments.
In light of these limitations, the experiments were discontinued.

**INCORRECT**
Understanding the effect of substituents on the parent molecules, the ortho hydrogens could be assigned to the high-frequency peak.

**CORRECT**
Understanding the effect of substituents on the parent molecules, we could assign the ortho hydrogens to the high-frequency peak.

**INCORRECT**
Using the procedure described previously, the partition function can be evaluated.

**CORRECT**
Using the procedure described previously, we can evaluate the partition function.

In some cases, the passive voice can be used to correct a dangling modifier.

**INCORRECT**
After combining the reactants, the reaction mixture was stirred at room temperature for 3 h.

**CORRECT**
After the reactants were combined, the reaction mixture was stirred at room temperature for 3 h.
INCORRECT
After stirring the mixture, 5 mg of compound 2 was added.

CORRECT
After the mixture was stirred, 5 mg of compound 2 was added.

➤ Phrases starting with “based on” must modify a noun or pronoun that usually immediately precedes or follows the phrase. Use phrases starting with “on the basis of” to modify a verb.

INCORRECT
Based on resonance enhancement and frequency shifts, changes in the inter-ring separation were calculated.

CORRECT
On the basis of resonance enhancement and frequency shifts, changes in the inter-ring separation were calculated.

INCORRECT
Based on extensive study, this genetic deficiency was attributed to the loss of one isozyme. (“Based on extensive study” modifies the noun “deficiency”, but this is not the meaning.)

CORRECT
On the basis of extensive study, this genetic deficiency was attributed to the loss of one isozyme. (“On the basis of extensive study” modifies the verb “was attributed.”)

Style guidelines based on authoritative sources are included in this book. (“Based on authoritative sources” modifies the noun “guidelines”.)

➤ “Due to” means “attributable to”; use it only to modify a noun or pronoun directly preceding it in the sentence or following a form of the verb “to be”.

INCORRECT
Delays resulted due to equipment failure.

CORRECT
Delays due to equipment failure resulted.
The delays were due to equipment failure.

INCORRECT
This high value resulted due to the high conversion efficiencies of the enzymatic reactor.
This high value is due to the high conversion efficiencies of the enzymatic reactor.

This high value resulted from the high conversion efficiencies of the enzymatic reactor.

Due to exposure to low levels of lead, children can be at risk for developmental problems.

Because of exposure to low levels of lead, children can be at risk for developmental problems.

Children can be at risk for developmental problems because of exposure to low levels of lead.

Absolute constructions are words, phrases, or clauses that are grammatically unconnected with the rest of the sentence in which they appear. They are sometimes called “sentence modifiers” because they qualify the rest of the sentence. They may occur anywhere in the sentence, and they are always set off by commas. They are not dangling modifiers.

Contrary to the excited-state situation, metal–metal bonding interactions in the ground states are weak.

The conclusions were premature, considering the lack of available data.

Judging from the spectral changes, exhaustive photolysis of compound 4 had occurred.

The conformations about the Re–Re bond, in addition, are different for all three complexes.

When necessary, the solutions were deaerated by bubbling nitrogen.

Clearly, alternative synthetic methods are possible.

The instructor having made her point, the discussion continued.

Absolute constructions often begin with one of the following words:

- concerning
- considering
- failing
- given
- judging
- provided
- providing
- regarding

- In mathematical papers, absolute phrases beginning with the words “assuming” and “taking” are often used as sentence modifiers.

Assuming that distance \( d \) is induced by the norm, \( M \) is a symmetrical and positively defined matrix.

Taking this value as an upper limit, the two shortest distances are sometimes too long for incipient hydrogen bonds.
• A subordinate or elliptical clause may be used as a sentence modifier.
The compound is stable in air, as we concluded from the experimental evidence.
The Mo 5s orbitals, as expected, interact strongly with the ligands.

• An introductory infinitive or infinitive phrase may be a sentence modifier.
To prepare compound 2, the method of Garner was followed.

Reflexive Pronouns

➤ Use the reflexive pronouns “myself”, “yourself”, “himself”, “herself”, “itself”, “ourselves”, and “themselves” only to refer back to a noun or another pronoun in the same sentence.

INCORRECT
Please send your manuscript to the associate editor or myself.

CORRECT
Please send your manuscript to the associate editor or me.
The associate editor herself will review your manuscript.

INCORRECT
My collaborators and myself will evaluate the results.

CORRECT
My collaborators and I will evaluate the results.
I will evaluate the results myself.
I myself will evaluate the results.

Punctuation

Comma

➤ Use a comma before, but not after, the coordinating conjunctions “and”, “or”, “nor”, “but”, “yet”, “for”, and “so” connecting two or more main clauses (complete thoughts).

Toluene and hexane were purified by standard procedures, and benzene was redistilled from calcium hydride.
The role of organic templates in zeolite synthesis has been studied extensively, but no general principles have been delineated.
Supported metals are among the most important industrial catalysts, yet only a few have been studied thoroughly.
No dielectric constants are available for concentrated acids, so it is difficult to give a quantitative explanation for the results.
Use a comma after a subordinate clause that precedes the main clause in a complex sentence.

Although 40 different P450 enzymes have been identified, only six are responsible for the processing of carcinogens.

Since the institute opened, plant breeders have developed three new prototypes.

Because the gene and the molecular marker are so close on the chromosome, they segregate together in the progeny.

Use a comma after most introductory words and phrases.

However, the public is being inundated with stories about cancer-causing chemicals.

Therefore, the type of organic solvent used is an important factor in lipase-catalyzed enzymatic synthesis.

After 3 months, the plants grown under phosphorus-deficient conditions were evaluated.

Thus, their motion is the result of the rotation of ferromagnetic domains.

On cooling, a crystalline phase may develop in coexistence with an amorphous phase.

Use a comma before the coordinating conjunction in a series of words, phrases, or clauses of equal rank containing three or more items. (This comma is called the *serial comma*.)

Water, sodium hydroxide, and ammonia were the solvents.

The red needles were collected, washed with toluene, and dried in a vacuum desiccator.

The compound does not add bromine, undergo polymerization by the Diels–Alder reaction, or react with electrophiles.

In compound sentences containing coordinating conjunctions, the clause following the conjunction is punctuated as if it were alone.

The reaction proceeds smoothly, and by use of appropriate reagents, the yields will be enhanced.

The compounds were separated, and after the filters had been washed, the experiments were completed.

Do not use a comma to separate a verb from its subject, its object, or its predicate noun.

**INCORRECT**

The addition of substituted silanes to carbon–carbon double bonds, has been studied extensively.
CORRECT
The addition of substituted silanes to carbon–carbon double bonds has been studied extensively.

INCORRECT
The disciplines described in the brochure include, materials science, biotechnology, and environmental chemistry.

CORRECT
The disciplines described in the brochure include materials science, biotechnology, and environmental chemistry.

INCORRECT
The solvents used in this study were, cyclohexane, methanol, n-pentane, and toluene.

CORRECT
The solvents used in this study were cyclohexane, methanol, n-pentane, and toluene.

➤ Do not use a comma before the conjunction joining a compound predicate consisting of only two parts.

INCORRECT
The product distribution results were obtained in sodium hydroxide, and are listed in Table 10.

CORRECT
The product distribution results were obtained in sodium hydroxide and are listed in Table 10.

➤ Use commas to separate items in a series that contains another series in parentheses already separated by commas.

The structure was confirmed with spectroscopy (1H NMR, UV, and IR), high-resolution mass spectrometry, and elemental analysis.

➤ Use a comma between two or more adjectives preceding a noun only if you can reverse the order of the adjectives without losing meaning. If you can insert the word “and”, the comma is correct.

The intense, broad signals of the two groups confirmed their location.
The broad, intense signals of the two groups confirmed their location.

Sample preparation is a repetitious, labor-intensive task.
Sample preparation is a labor-intensive, repetitious task.

A powerful, versatile tool for particle sizing is quasi-elastic light scattering.
A versatile, powerful tool for particle sizing is quasi-elastic light scattering.
But:

Polyethylene is an important industrial polymer.
The rapid intramolecular reaction course leads to ring formation.
The backbone dihedral angles were characterized by $J$ couplings.
The local structural environment of the Mn cluster was determined.

➤ Use a comma before, but not after, the subordinating conjunction in a nonrestrictive clause.

INCORRECT

The bryopyran ring system is a unique requirement for anticancer activity whereas, the ester substituents influence the degree of cytotoxicity.

CORRECT

The bryopyran ring system is a unique requirement for anticancer activity, whereas the ester substituents influence the degree of cytotoxicity.

➤ Use commas to set off nonrestrictive phrases or clauses.

The products, which were produced at high temperatures, were unstable.

➤ Phrases introduced by “such as” or “including” can be restrictive (and thus not set off by commas) or nonrestrictive (and thus set off by commas).

Potassium compounds such as KCl are strong electrolytes; other potassium compounds are weak electrolytes.
Previously, we described a mathematical model including a description of chlorophyll degradation in foods.
Divalent metal ions, such as magnesium(II) and zinc(II), are located in the catalytic active sites of the enzymes.
Hydrogen-bonded complexes, including proton-bound dimers, are well-known species.

In the first two sentences, the phrases are restrictive because the sentences do not make their points without the phrases. In the third and fourth sentences, the phrases are nonrestrictive because the sentences can make their points without the phrases.

➤ An appositive is a noun that follows another noun and identifies or explains the meaning of the first noun.

My wife, Jeanne, is a biochemist at the National Institutes of Health.
My son James plays baseball, and my son John plays soccer.

An appositive is nonrestrictive (and therefore set off by commas) when it names the only possibility. In the first sentence, Jeanne is a nonrestrictive appositive. An
appositive is restrictive (and therefore not set off by commas) when it points out one of two or more possibilities. In the second sentence, the names of the two sons are restrictive appositives.

➤ Use commas to set off the words “that is”, “namely”, and “for example” when they are followed by a word or list of words and not a clause. Also use a comma after the item or items being named. Use a comma after “i.e.” and “e.g.” in parenthetical expressions.

The new derivatives obtained with the simpler procedure, that is, reaction with organocuprates, were evaluated for antitumor activity.

Alkali metal derivatives of organic compounds exist as aggregates of ion pairs, namely, dimers, trimers, and tetramers, in solvents of low polarity.

Many antibiotics, for example, penicillins, cephalosporins, and vancomycin, interfere with bacterial peptidoglycan construction.

These oxides are more stable in organic solvents (e.g., ketones, esters, and ethers) than previously believed.

➤ Use commas to separate two reference citation numbers, but use an en dash (–) to express a range of three or more in sequence, whether they are superscripts or are on the line in parentheses. When they are superscripts, do not use a space after the comma.

Experimental investigations\textsuperscript{10,14,18–25} concerned the relative importance of field and electronegativity effects.

Certain complexes of cobalt were reported (10, 11) to have catalytic effects on hydrolysis reactions.

Flash photolysis studies (3–7) demonstrated the formation of transient intermediate products such as triplet states.

➤ Use a comma before Jr. and Sr., but treat II and III according to the person’s preference. Within a sentence, always use a comma after Jr. and Sr., but use a comma after II and III only if they are preceded by a comma.

William M. Delaney, Jr.
Charles J. Smith, III
John J. Alden II

William M. Delaney, Jr., was elected to the governing board.

Charles J. Smith, III, received a majority of the votes.

John J. Alden II did not run for office this year.

➤ Do not use a comma preceding “et al.” unless commas are needed for other reasons.
In dates, use a comma after the day, but not after the month when the day is not given.

June 15, 1996
June 1996

When giving a complete date within a sentence, use a comma after the year as well.

On August 18, 1984, an extraordinary person was born.

When a geographical location is named within a sentence and the name includes a comma, use a comma at the end of the name as well.

Iona College, in New Rochelle, New York, is the CEO’s alma mater.

The lead researcher, who obtained her education at the University of Calgary, Alberta, Canada, addressed the reporters’ questions.

Use a comma to introduce quotations.

In the words of Pasteur, “Chance favors the prepared mind.”

Pasteur said, “Chance favors the prepared mind.”

Do not use a comma after a quotation that is the subject of the sentence.

“Chance favors the prepared mind” is a translation from the French. (The quotation is the subject of the sentence.)

**Period**

Use a period at the end of a declarative sentence, but never in combination with any other punctuation marks.

He said, “Watch out!”

She asked, “May I go?”

Do not use periods after most abbreviated units of measure, except when the abbreviation could be confused with a word (in. for inches, at. for atomic, no. for number).

If a sentence ends with an abbreviation that includes a period, do not add another period.

She will return at 3 a.m.
➤ Use periods and spaces after initials in persons’ names.

J.-L. Gay Lussac       J. E. Lennard-Jones       M. S. Newman

**EXCEPTION** Use periods but no spaces when referring to authors of a paper in the acknowledgment paragraph of the paper.

R.C.McD. and C.R. thank Dr. Rose Allan for carefully reading the manuscript.

C.-C.Y., L.B.-P., N.-h.X., and S.Zh.O. are grateful for generous support from the university.

➤ Do not use periods in abbreviations or acronyms of institution or organization names.

ACS          CNRS          NASA          NIH

**Semicolon**

➤ Use a semicolon to separate independent clauses that are not joined by a conjunction.

All solvents were distilled from an appropriate drying agent; tetrahydrofuran and diethyl ether were also pretreated with activity I alumina.

➤ Use semicolons between items in a series of words, phrases, or data strings if one or more of the items already contain commas.

We thank Zachary Axelrod, University of Michigan, for spectral data; Caroline Fleissner, Harvard University, for helpful discussions; and the National Science Foundation for financial support (Grant XYZ 123456).

The product was dried under vacuum to give compound 2: yield 68%; IR 1991 m, 1896 s, sh, 1865 s cm\(^{-1}\); \(^1\)H NMR 0.36 ppm; \(^{13}\)C NMR 221.3, 8.1 ppm.

Figure 1. Cyclic voltammograms in dichloromethane: (a) compound 1, 23 °C; (b) compound 2, –40 °C; (c) compound 4, 23 °C.

Figure 6. Ru–H stretches in the IR spectrum of compound 5: ×, 298 K; +, 90 K.

This rule holds even if the only group containing the commas is the last in the series.

The compounds studied were methyl ethyl ketone; sodium benzoate; and acetic, benzoic, and cinnamic acids.

➤ Use a semicolon between independent clauses joined by conjunctive adverbs or transitional phrases such as “that is”,” however”, “therefore”, “hence”, “indeed”, “accordingly”, “besides”, and “thus”.

The rate at which bleaching occurred was dependent on cluster size; that is, the degradation of the mononuclear cluster was about 5 times faster than that of the tetranuclear cluster.
Many kinetic models have been investigated; however, the first-order reactions were studied most extensively.

The proposed intermediate is not easily accessible; therefore, the final product is observed initially.

The restriction of the rotational motions of the tert-butyl group gives rise to large entropy changes for the association reaction; hence, the covalent form is relatively easy to identify.

The efficiency of the cross-coupling depends on the nature of X in RX; thus, the reaction is performed at room temperature by slow addition of the ester.

Do not use a semicolon between dependent and independent clauses.

**Incorrect**

The activity on bromopyruvate was decreased; whereas, the activity on pyruvate was enhanced.

**Correct**

The activity on bromopyruvate was decreased, whereas the activity on pyruvate was enhanced.

**Colon**

Use a colon to introduce a word, a phrase, a complete sentence, or several complete sentences that illustrate, clarify, or expand the information that precedes it. Capitalize the first word after a colon only if the colon introduces more than one complete sentence, a quotation, or a formal statement.

The electron density was studied for the ground state of three groups of molecules: (1) methane–methanol–carbon dioxide, (2) water–hydrogen peroxide, and (3) ferrous oxide–ferric oxide.

We now report a preliminary finding: no chemical shift changes were detected in the concentration range 0.1–10 M.

The following are our conclusions: Large-angle X-ray scattering studies give us an accurate picture of structures up to 9 Å. They do not allow the specification of defects, such as random ruptures of the chains. The structural models defined are strongly supported by magnetic measurements.

In figure captions, use a colon to introduce explanations of symbols or other aspects of the figure.

**Figure 1.** Variable-temperature \(^1\)H NMR spectra of compound 12: top, 403 K; middle, 353 K; bottom, 298 K.

**Figure 3.** Brønsted-type plots for aminolysis in 1 M KCl at 25 °C: ○, 2-nitrophenyl acetate; □, 3-chlorobenzoic acid; ◇, 2,6-dinitrobenzoic acid.
Do not use a colon (or any punctuation) between a verb and its object or complement or between a preposition and its object.

**INCORRECT**

The rate constants for the reaction in increasing concentrations of sodium hydroxide are: 3.9, 4.1, 4.4, 4.6, and 4.9.

**CORRECT**

The rate constants for the reaction in increasing concentrations of sodium hydroxide are 3.9, 4.1, 4.4, 4.6, and 4.9.

**INCORRECT**

The thermal decomposition was investigated with: gas chromatography, BET surface areas, and X-ray powder diffraction.

**CORRECT**

The thermal decomposition was investigated with gas chromatography, BET surface areas, and X-ray powder diffraction.

**INCORRECT**

Transition-metal nitrides have many properties that make them suitable for industrial applications, including: high wear resistance, high decomposition temperature, and high microhardness.

**CORRECT**

Transition-metal nitrides have many properties that make them suitable for industrial applications, including high wear resistance, high decomposition temperature, and high microhardness.

Use either a colon or a slash to represent a ratio, but not an en dash. Use either a slash or an en dash between components of a mixture, but not a colon.

- dissolved in 5:1 glycerin/water
- dissolved in 5:1 glycerin–water
- the metal/ligand (1:1) reaction mixture
- the metal–ligand (1:1) reaction mixture
- the metal–ligand (1/1) reaction mixture
- the methane/oxygen/argon (1/50/450) matrix
- the methane/oxygen/argon (1:50:450) matrix

**Quotation Marks**

Location of closing quotation marks with respect to other punctuation is a style point in which ACS differs from other authorities. In 1978, ACS questioned the traditional practice and recommended a deviation: logical placement. Thus, if the punctuation is part of the quotation, then it should be within the quotation marks.
marks; if the punctuation is not part of the quotation, the writer should not mislead the reader by implying that it is.

➤ Place closing quotation marks before all punctuation that is not part of the original quotation. Place them after all punctuation that is part of the quotation.

The sample solution was stirred briefly with a magnetic “flea”.
Ralph Waldo Emerson said, “The reward of a thing well done is to have done it.”

➤ Use quotation marks around words used in a new sense or words not used literally, but only the first time they appear in text.

Plastocyanin is a soluble “blue” copper protein.

The integrated intensity of each diagonal in the spectrum is proportional to a “mixing coefficient”.

The “electron-deficient” cations are, in fact, well-established intermediates.

➤ Use quotation marks to enclose the titles of uniquely named parts and sections of a book or a paper.

A complete description of the oils is given in the section “Flavonoids in Citrus Peel Oils”, and other references are listed in the bibliography.

But:

The preface describes the complexity of the problem.

➤ Use quotation marks to enclose short direct quotations (up to three sentences).

In the book Megatrends, Naisbitt concludes, “We are moving from the specialist who is soon obsolete to the generalist who can adapt.”

➤ Use a narrower column width (that is, indented on both sides) for longer quotations (extracts) of 50 words or more. Do not use quotation marks.

Everything is made of atoms. That is the key hypothesis. The most important hypothesis in all of biology, for example, is that everything that animals do, atoms do. In other words, there is nothing that living things do that cannot be understood from the point of view that they are made of atoms acting according to the laws of physics.
—Richard Phillips Feynman

However, this convention does not apply in an article quoting someone who has been interviewed. In such cases, quoted text need not be differentiated by column width, and quotation marks should be used.

➤ Use single quotation marks only when they are within double quotation marks.

He said, “You should read the article ‘Fullerenes Gain Nobel Stature’ in the January 6, 1997, issue of Chemical & Engineering News.”
**Parentheses**

Parenthetical expressions contain information that is subsidiary to the point of the sentence. The sentence does not depend on the information within the parentheses.

➤ Use parentheses for parenthetical expressions that clarify, identify, or illustrate and that direct the reader.

- The total amount (10 mg) was recovered by modification of the procedure.
- The final step (washing) also was performed under a hood.
- The curve (Figure 2) obeys the Beer–Lambert law.
- The results (Table 1) were consistently positive.
- Only 15 samples (or 20%) were analyzed.

➤ Punctuate after, not before, parenthetical expressions.

**Incorrect**

- Compound 1, (7 mg) obtained by typical workup methods, was used without further purification.

**Correct**

- Compound 1 (7 mg), obtained by typical workup methods, was used without further purification.

➤ If a parenthetical sentence is within another sentence, do not use a final period within the closing parenthesis, and do not start the parenthetical sentence with a capital letter.

- Our results (the spectra are shown in Figure 5) justified our conclusions.
- Our results justified our conclusions (the spectra are shown in Figure 5).

➤ If a parenthetical sentence is not within another sentence, use a final period inside the closing parenthesis, and start the parenthetical sentence with a capital letter.

- A mechanism involving loss of a CH radical followed by rearrangement was proposed. (The reactions are shown in Scheme 1.)

➤ Use parentheses to enclose numerals in a list. Always use parentheses in pairs, not singly.

- Three applications of this reaction are possible: (1) isomerization of sterically hindered aryl radicals, (2) enol–keto transformation, and (3) sigmatropic hydrogen shift.
Use parentheses to identify the manufacturer of reagents and equipment.

- cobalt chloride (Mallinckrodt)
- a pH meter with a glass electrode (Corning)

Do not use parentheses when citing a reference number in narrative text. In such a case, the reference number is the point of the sentence, not subsidiary information, and thus not parenthetical.

**INCORRECT**

- in ref (12), in (12)

**CORRECT**

- in ref 12

Use parentheses in mathematical expressions as discussed in Chapter 11 and in chemical nomenclature and notation as discussed in Chapters 12 and 13.

**Square Brackets**

Use square brackets within quotation marks to indicate material that is not part of a direct quote.

In the words of Sir William Lawrence Bragg, “The important thing in science is not so much to obtain new facts as to *discover new ways* [italics added] of thinking about them.”

Use square brackets to indicate concentration: \([\text{Ca}^+]\). 

Use square brackets in mathematical expressions as discussed in Chapter 11 and in chemical nomenclature and notation as discussed in Chapters 12 and 13.

**Dashes**

The shortest dash is the hyphen (−); the en dash (–) is longer; and the em dash (—is the longest. Hyphens are discussed in the section on hyphenation in Chapter 10, starting on p 135.

**En Dash**

Use an en dash to mean the equivalent of “and”, “to”, or “versus” in multiword concepts where the words are of equal weight.

- acid–base titration
- bromine–olefin complex
- carbon–oxygen bond
- cis–trans isomerization
- cost–benefit analysis
- dose–response relationship
- ethanol–ether mixture
- freeze–pump–thaw degassed
- helix–coil transition
- host–guest complexation
log–normal function
metal–ligand complex
metal–metal bonding
nickel–cadmium battery
oxidation–reduction potential
producer–user communication
pump–probe technique
red–black dichroic crystals
structure–activity relationship
structure–property relationship
temperature–time curve
vapor–liquid equilibrium
winter–fall maxima
0–∞ sequence

**EXCEPTION** Use a hyphen for color combinations such as blue-green. See Chapter 10, page 140.

➤ Use an en dash to mean “to” or “through” with a span of three or more numerals or other types of ranges.

- 12–20 months
- Figures 1–4
- 5–50 kg
- sections 1b–1f
- parts C–E
- compounds A–I
- Lyon and co-workers (23–26)
- Lyon and co-workers23a–d

**EXCEPTION 1** When either one or both numbers are negative or include a symbol that modifies the number, use the word “to” or “through”, not the en dash.

- –20 to +120 K
- –145 to –30 °C
- ≈50 to 60
- 10 to >600 mL
- <5 to 15 mg

**EXCEPTION 2** Do not use an en dash when the word “from” or “between” is used.

- from 500 to 600 mL (not from 500–600 mL)
- between 7 and 10 days (not between 7–10 days)

➤ Use an en dash to link the names of two or more persons of equal importance used as a modifier.

- Bednorz–Müller theory
- Beer–Lambert law
- Bose–Einstein statistics
- Debye–Hückel theory
- Diels–Alder reaction
- Fermi–Dirac statistics
- Fischer–Tropsch effect
- Fisher–Johns hypothesis
- Flory–Huggins interaction
- Franck–Condon factor
- Friedel–Crafts reaction
- Geiger–Müller effect
- Henderson–Hasselbalch equation
- Jahn–Teller effect
- Lee–Yang–Parr method
- Lineweaver–Burk method
- Mark–Houwink plot
- Meerwein–Ponndorf theory
- Michaelis–Menten kinetics
- Stern–Volmer plot
- van’t Hoff–Le Bel theory
- Wolff–Kishner theory
- Young–Laplace equation
- Ziegler–Natta-type catalyst

Treatment of double surnames is covered in Chapter 10 (p 139).
Use an en dash between components of a mixed solvent. (A slash can also be used.)

The melting point was unchanged after four crystallizations from hexane–benzene.

**Em Dash**

Use em dashes to set off words that would be misunderstood without them.

**INCORRECT**

All three experimental parameters, temperature, time, and concentration, were strictly followed.

**CORRECT**

All three experimental parameters—temperature, time, and concentration—were strictly followed.

Do not use em dashes to separate phrases or nonrestrictive clauses if another form of punctuation can be used.

**INCORRECT**

Knauth—not Stevens—obtained good correlation of results and calculations.

**CORRECT**

Knauth, not Stevens, obtained good correlation of results and calculations.

**INCORRECT**

The singly charged complexes—which constituted bands 1 and 3—liberated maleate anion upon decomposition.

**CORRECT**

The singly charged complexes, which constituted bands 1 and 3, liberated maleate anion upon decomposition.

**Ellipsis Points**

Within a quotation, use three periods (points of ellipsis) to indicate deleted words or phrases. These three periods are in addition to other needed punctuation. Thus, if a period is already there, the result will be four periods.

No science is immune to the infection of politics and the corruption of power.... The time has come to consider how we might bring about a separation, as complete as possible, between Science and Government in all countries.

—Jacob Bronowski

Do not begin or end a quotation with ellipsis points.
➤ Use ellipsis points where part of a series is omitted, when the pattern of the series is unambiguous.

\[ a = 1, 2, 3, \ldots \]
\[ n = 2, 4, 6, \ldots \]
\[ x = 1, 3, 5, \ldots, 15 \]

**Spelling**

Consult a dictionary to resolve spelling questions. *Merriam-Webster’s Collegiate Dictionary* and *Webster’s New World College Dictionary* are the desk dictionaries used by the ACS technical editing staff. ACS staff members also use the unabridged *Webster’s Third New International Dictionary*. However, whatever your dictionary, choose the first spelling of a word. Use American spellings, except in proper names and direct quotations (including titles). Appendix 9-1 contains a list of the recommended spellings for words that have two or more acceptable spellings.

➤ For the correct spelling and styling of company names, search the Internet for the company and look for the company name on its “contact” page. Do not rely on either a company’s home page or the presence of a particular spelling in a search engine, because the former may be informal and the latter common but also incorrect.

**Tricky Possessives**

➤ Form the possessive of a joint owner by adding an apostrophe and an “s” after the last name only.

Celapino and Marshall’s results
Bausch and Lomb’s equipment

➤ Form the possessive of plural nouns that do not end in “s” by adding an apostrophe and an “s”. Form the possessive of plural nouns that end in “s” by adding an apostrophe only.

people’s rights
children’s books
compounds’ structures

➤ Form the possessive of a proper name ending in “s” by adding an apostrophe and an “s”.

Jacobs’s laboratory
Mathers’s reception
**Tricky Plurals**

Sometimes, the plural form is so familiar that it is used erroneously instead of the singular, usually with Latin and other non-English words. The following list shows the correct singulars and plurals. The preferred forms are given first.

<table>
<thead>
<tr>
<th>SINGULAR</th>
<th>PLURAL</th>
</tr>
</thead>
<tbody>
<tr>
<td>alga</td>
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<td>appendixes, appendices</td>
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<td>helixes, helices</td>
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<td>hypotheses</td>
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<td>index</td>
<td>indexes</td>
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<td>latices, latexes</td>
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<td>loci</td>
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<td>vertex</td>
<td>vertexes, vertices</td>
</tr>
<tr>
<td>vortex</td>
<td>vortexes, vortices</td>
</tr>
</tbody>
</table>
APPENDIX 9-1

Recommended Spelling List

Many words in regular usage, as well as many technical terms, have two or more acceptable spellings. The following list gives recommended spellings and capitalizations, where appropriate, for some terms not found in easily accessible dictionaries, words often misspelled, common expressions, and words for which the ACS preference may not match your dictionary’s.

- absorbance
- absorbency
- absorbent
- accommodate
- acknowledgment
- adsorbent
- aerobic
- aging
- aglycon
- air-dry (verb)
- ambiguous
- amine (RNH₂)
- ammine (NH₃ complex)
- amphiphile
- ampule
- analog (computer)
- analogue (structural derivative)
- analyte
- analyze
- annelation
- annulation
- antioxidant
- appendixes
- aqua regia
- Arrhenius
- artifact
- asymmetry
- audio frequency
- autoxidation
- auxiliary
- Avogadro
- bacitracin
- back-bonding
- back-donation
- back-titrate (verb)
- backscatter
- backscattering
- backward
- band gap
- bandwidth
- baseline
- Beckmann (thermometer, rearrangement)
- Beer’s law
- Beilstein
- bit
- black box
- blackbody
- blender
- Boltzmann
- borderline
- Bragg scattering
- break-seal
- break up (verb)
- breakup (noun)
- bremsstrahlung
- bridgehead
- broad band (noun)
- broad-band (adjective)
- Brønsted
- Büchner
- build up (verb)
- buildup (noun)
- buret
- butanol, 1-butanol (not n-butanol)
n-butyl alcohol
cut off (verb)
tert-butylation
cutoff (noun)
byline
cuvette
bypass
cytochrome c
byp product
deamino (not desamino)
byte
deoxy (not desoxy)
canceled
dependent
canister
desiccator
cannot
desamine (amino acid names only)
Cartesian
deuterioxide
catalog
deuteroporphyrin
catalog
Dewar benzene
catalog
Dewar flask
clean up (verb)
dialogue
cleanup (noun)
diffractometer
clear-cut
disc (electrophoresis, compact disc)
co-occurrence
discernible
closed up (noun)
discernible
closure (n)
distill
co-occurrence
distill
collinear
dry ice
colorimetric
drybox
collaborative
dyad
collinear
e-mail
colorimetric
ebullaoscopic
collinear
eigenfunction
collinear
eigenvalue
collinear
electroless
collinear
electron microscope
collinear
electronvolt
collinear
electrooptic
collinear
electropositive
collinear
eflu ent
collinear
eflu ent
Darzens
counter electrode
eflu ent
Darzens
counteranion
Elvehjem
counterion
end point
coverslip
elu ate
cross-coupling
eulent
cross-link
Elve him
cross over (verb)
Erlenmeyer (flask)
cross-react
exchangeable
cross-react
crossover (verb)
cross-reaction
cross-reaction
cross section (noun)
cross-section (adjective)
cross-reaction
crossover (noun, adjective)
cuboctahedron
fal l off (verb)
cuboctahedron
fal l off (noun, adjective)
far-infrared
faradic (referring to current, not the person)
fax (noun, verb, adjective)
feedback
fiber-optic (adjective)
fiber optics (noun)
filterable
firebrick
flavin
flow sheet
fluoroborate
fluoramine
fluoro amine
focused
follow up (verb)
follow-up (noun, adjective)
forbear (verb, to refrain)
forebear (noun, ancestor)
forego (verb, to go before)
foreword (part of a book)
forgo (verb, to do without)
formulas
forward (direction)
freeze-dry (verb)
fulfill
γ ray
gauge
Gaussian
genegenion
glovebag
glovebox
Gouy
graduated cylinder
gram
Gram-negative
Gram-positive
gray
Grignard
groundwater
half-ester
half-life
half-width
halfway
Hamiltonian
Hantzsch
hazmat
heat-treat (verb)
hemoglobin
hemolysate
heterogeneous
Hoffmann degradation
homogeneous
homologue
Hunsdiecker
hydrindan
hydriodic
hydriodide
hydrolysate
hydrolyzed
ice-cold
ice–water bath (use en dash, see p 124)
inasmuch
indan
indexes (book parts, catalog)
indices (mathematical)
indispensable
inflection
infrared
innocuous
inoculate
insofar
inter-ring
iodometric
iodometry
isoctane
isopiestic
isosbestic
isopropyl alcohol (not isopropanol)
isobestic
judgment
Karl Fischer
kayser
Kekulé
Kjeldahl
Kramers
Kugelrohr
labeled
laser
leukocyte
leveling
levorotatory
lifetime
ligancy
ligate
ligated
line shape
line width
liquefy
liter
lumiflavin
luster
lysate
lysed
make up (verb)
makeup (noun)
Markovnikov
matrices (mathematical)
matrixes (media)
megohm
Mendeleev
mesoporphyrin
metalate
metalation
metallization
metallize
metalloenzyme
meter
micro-Kjeldahl
mid-infrared
midpoint
minuscule
mixture melting point
monochromator
Mössbauer
naphthyl
near-ultraviolet
neopentyl
Nernstian
nuclide
occurred
occurrence
occurring
ortho ester
orthoformate
orthohydrogen
orthopositronium
outgas
outgassing
overall
parametrization
path length
percent
Petri
pharmacopeia
phenolphthalein
phlorin
phosphomonoester
phosphorous (as in phosphorous acid)
phosphorus (element)
phthalic
pipet
pipetted
plaster of Paris
point source
porphine
porphyrin
portland cement
programmed
2-propanol (not isopropanol)
pseudo-first-order
pyrolysate
quantitation
radio frequency
radioelement
radioiodine
radionuclide
re-form (to form again)
reform (to amend)
repellent
riboflavin
ring-expand (verb)
rotamer
scale up (verb)
scale-up (noun)
scavengeable
Schwarzkopf
seawater
self-consistent
selfsame
Sephadex
set up (verb)
setup (noun)
side arm (noun)
side chain  
sideband  
siphon  
Soxhlet  
spin-label (noun)  
spin–lattice (use en dash, see p 124)  
spin–orbit (use en dash, see p 124)  
steam bath  
steam-distill (verb)  
stepwise  
stereocenter  
stereopair  
stereoptically  
Student’s $t$ test or the Student $t$ test  
sulfolane  
sulfur  
superacid  
superhigh frequency  
supernatant (adjective)  
supernate (noun)  
syndet  
synthase  
synthetase  
test tube  
θ solvent  
thiamin  
thioacid  
thioester  
thioether  
thioketone  
toward  
transmetalation  
tropin  
Ubbelohde  
ultrahigh vacuum  
un-ionized  
uni-univalent  
upfield  
urethane  
vand der Waals  
VandenHeuvel  
vant Hoff–Le Bel (use en dash, see p 124)  
Vigreux  
vis-à-vis  
voltmeter (measures voltaic electricity)  
voltammetry (measures ranges of volts and amperes)  
voltmeter (measures cell potential)  
wastewater  
wave function  
waveform  
wavelength  
wavenumber  
well-known  
work up (verb)  
workup (noun)  
X-irradiation  
X-ray  
ylide  
zerovalent  
zigzag  
zinc blende
This chapter presents recommended stylistic and editorial conventions, mainly but not solely for ACS publications. The style recommended by ACS is, for the most part, taken from established authoritative sources, such as *The Chicago Manual of Style*, *Words into Type*, and the *United States Government Printing Office Style Manual*.

Other points of style are discussed in Chapter 11, “Numbers, Mathematics, and Units of Measure”; Chapter 12, “Names and Numbers for Chemical Compounds”; and Chapter 13, “Conventions in Chemistry”.

**Hyphenation**

Consult a dictionary to resolve hyphenation questions. *Merriam-Webster’s Collegiate Dictionary* and *Webster’s New World College Dictionary* are the desk dictionaries used by the ACS technical editing staff. ACS staff also use the unabridged *Webster’s Third New International Dictionary*.

**Prefixes**

Most prefixes are not hyphenated. Do not hyphenate the following prefixes when added to words that are not proper nouns.

<table>
<thead>
<tr>
<th>Prefixes</th>
<th>Prefixes</th>
<th>Prefixes</th>
<th>Prefixes</th>
</tr>
</thead>
<tbody>
<tr>
<td>after</td>
<td>bio</td>
<td>de</td>
<td>hetero</td>
</tr>
<tr>
<td>ante</td>
<td>by</td>
<td>di</td>
<td>homo</td>
</tr>
<tr>
<td>anti</td>
<td>co</td>
<td>down</td>
<td>hyper</td>
</tr>
<tr>
<td>auto</td>
<td>counter</td>
<td>electro</td>
<td>hypo</td>
</tr>
<tr>
<td>bi</td>
<td>cyber</td>
<td>extra</td>
<td>in</td>
</tr>
</tbody>
</table>
infra infra
inter mini mid
intra mis mis
intro mono mono
iso multi multi
macro nano nano
mega neo neo
meso non non
meta over over
metalla peri peri
metallo photo photo
micro physico physico
infra infra 
inter mini mid
intra mis mis
intro mono mono
iso multi multi
macro nano nano
mega neo neo
meso non non
meta over over
metalla peri peri
metallo photo photo
micro physico physico

**EXAMPLES**

- antibacterial
- isospin
- precooled
- cooperation
- microorganism
- pseudomorph
- cyberspace
- multicolored
- superacid
- extranuclear
- non-polar
- transactinide
- interelectrode
- photoredox
- viscoelastic

**EXAMPLES**

- anti-infective
- inter-ring
- post-reorganization
- anti-inflammatory
- intra-ring
- post-translational
- bi-univalent
- mid-infrared
- pre-equilibrium
- co-ion
- non-native
- sub-bandwidth
- co-worker
- non-nuclear
- un-ionize

**Some prefixes may be hyphenated or not, depending on meaning.**

- recollect or re-collect
- recover or re-cover
- reform or re-form
- retreat or re-treat

**RARE EXCEPTIONS**

- autoxidation
- counter electrode
- hetero group
- homo nucleoside

**Do not hyphenate multiplying prefixes.**

- hemi, mono, di, tri, tetra, penta, hexa, hepta, octa, ennea, nona, deca, deka, undeca, dodeca, etc.
- semi, uni, sesqui, bi, ter, quadri, quater, quinque, sexi, septi, octi, novi, deci, etc.
- bis, tris, tetrakis, pentakis, hexakis, heptakis, octakis, nonakis, decakis, etc.
EXAMPLES

- 2,2’-bipyridine
- 1,4-bis(3-bromo-1-oxopropyl)piperazine
divalent
hemihydrate
heptacoordinate tetrahedron
hexachlorobenzene
1,1′:3′,1″:3″,1′′′-quaterphenyl
tetrakis(hydroxymethyl)methane
triatomic
triethyl phosphate
tris(ethylenediamine)cadmium dihydroxide

➤ Hyphenate a prefix to a two-word compound.

- multi-million-dollar lawsuit
- non-diffusion-controlled system
- non-English-speaking colleagues
- non-radiation-caused effects
- non-tumor-bearing organ
- pre-steady-state condition
- pseudo-first-order reaction

➤ Hyphenate prefixes to chemical terms.

- non-alkane
- non-phenyl atoms

➤ Hyphenate a prefix to a numeral.

- pre-1900s

➤ Hyphenate prefixes to proper nouns and adjectives, and retain the capital letter.

- anti-Markovnikov
- non-Coulombic
- non-Gaussian
- non-Newtonian
- oxy-Cope

Suffixes

➤ Most suffixes are not hyphenated. Do not hyphenate the following suffixes when added to words that are not proper nouns.

- able
- fold
- ful
- less
- like
- ment
- ship
- wide
- wise
Hyphenate the suffixes “like” and “wide” when they are added to words of three or more syllables.

- bacteria-like
- radical-like
- university-wide
- computer-like
- resonance-like

Hyphenate the suffix “like” in two-word compounds used as unit modifiers.

- first-order-like
- ion-exchange-like
- rare-earth-like
- transition-metal-like

Hyphenate the suffix “like” to chemical names.

- adamantane-like
- cycloalkane-like
- morphine-like
- olefin-like

Hyphenate a numeral and a suffix.

- 10-fold
- 25-fold

Hyphenate suffixes to proper nouns, and retain the capital letter.

- Asia-wide
- Claisen-like
- Kennedy-like
- Michaelis–Menten-like

**Compound Words**

Compound words are two or more terms used to express a single idea. Compound words in common usage are listed in most dictionaries. Many are hyphenated, but many are not.

- back-reaction
- cross-link
- half-life
- cross hairs
- crosshatch
- self-consistent
Hyphenate spelled-out fractions.

one-half
one-ninth
three-fourths
two-thirds

Hyphenate two-word verbs.

air-dry freeze-dry ring-expand
flame-seal jump-start vacuum-dry

Do not hyphenate phrasal verbs. As unit modifiers or nouns, these words are often hyphenated or closed up; check a dictionary.

break down mix up stand by
build up scale up take off
grow up set off warm up
hand out set up wear out
line up slow down

Do not hyphenate foreign phrases used as unit modifiers.

ab initio calculation
ad hoc committee
in situ evaluation
in vivo reactions

Some foreign phrases are hyphenated in the original language, for example, laissez-faire.

People who have double surnames may choose to hyphenate them or use a space between them. When they are hyphenated, use a hyphen, not an en dash, between the two surnames in a person’s name. Some combinations of two given names are also hyphenated.

Robert Baden-Powell  Joseph-Louis Gay-Lussac
David Ben-Gurion  Irene Joliot-Curie
Cecil Day-Lewis  Jackie Joyner-Kersee
Chen-Chou Fu  John Edward Lennard-Jones

Unit Modifiers

Unit modifiers are two words that together describe a noun; they are almost always hyphenated. Most unit modifiers consist of

- a noun and an adjective (e.g., time-dependent reaction, radiation-sensitive compound, water-soluble polymer, halogen-free oscillator);
- an adjective and a noun (e.g., high-frequency transition, small-volume method, first-order reaction, outer-sphere redox couple);
• an adjective and a participle (e.g., slow-growing tree, broad-based support, far-reaching influence);
• a noun and a participle (e.g., time-consuming project, earth-shaking news, silver-coated electrode);
• an adverb and an adjective (e.g., above-average results, still-unproven technique); or
• two nouns (e.g., ion-exchange resin, liquid-crystal polymers, transition-state modeling, charge-transfer reaction, gas-phase hydrolysis).

The following is a short list (by no means complete) of unit modifiers commonly seen in ACS publications. These should be hyphenated when modifying a noun.

- air-dried
- air-equilibrated
- back-bonding
- 14C-labeled
- charge-transfer
- cost-effective
- diffusion-controlled
- double-bond
- electron-diffraction
- electron-transfer
- energy-transfer
- excited-state
- first-order
- flame-ionization
- free-energy
- free-radical
- gas-phase
- gel-filtration
- Gram-negative
- Gram-positive
- halogen-free
- high-energy
- high-frequency
- high-performance
- high-pressure
- least-squares
- light-catalyzed
- long-chain
- long-lived
- low-energy
- low-frequency
- low-pressure
- low-resolution
- moisture-sensitive
- nearest-neighbor
- oil-soluble
- outer-sphere
- radiation-caused
- radiation-produced
- radiation-sensitive
- rate-limiting
- reversed-phase
- room-temperature
- round-bottom
- rubber-lined
- second-harmonic
- second-order
- side-chain
- size-dependent
- small-volume
- solid-phase
- solid-state
- species-specific
- steady-state
- structure-specific
- temperature-dependent
- thin-layer
- three-dimensional
- three-phase
- time-dependent
- transition-metal
- transition-state
- two-dimensional
- vapor-phase
- water-soluble
- weak-field
- wild-type

**EXCEPTIONS**

- particle size distribution
- water gas shift

➤ Hyphenate combinations of color terms used as unit modifiers.

- blue-green solution
- red-black precipitate
- bluish-purple solid
- silver-gray body
Do not hyphenate unit modifiers if the first word is an adverb ending in “ly”.

- accurately measured values
- carefully planned experiment
- poorly written report
- recently developed procedure

Hyphenate unit modifiers containing the adverbs “well”, “still”, “ever”, “ill”, and “little”.

- ever-present danger
- ever-rising costs
- ill-fitting stopper
- little-known hypothesis
- still-new equipment
- well-known scientist
- well-trained assistants

**EXCEPTION** Do not hyphenate unit modifiers containing the adverbs “well”, “still”, “ever”, “ill”, and “little” if they are modified by another adverb.

- most ill advised investment
- very high density lipoprotein
- very well studied hypothesis

Hyphenate unit modifiers containing a comparative or superlative if the meaning could be different without the hyphen.

- best-known processes
- best-loved advisor
- higher-temperature values
- least-squares analysis
- lowest-frequency wavelengths
- nearest-neighbor interaction

Do not hyphenate a number and a unit of time or measure used as a unit modifier.

- $1.2 \times 10^{-4}$ cm$^{-1}$ peak
- 25 K increments
- 10 mg sample
- a 0.1 mol dm$^{-3}$ solution
- 20 mL aliquot
- 12° angle

When two or more unit modifiers with the same ending base modify one noun, use a hyphen after each element, and do not repeat the ending base.

- first- and second-order reactions
- high-, medium-, and low-frequency measurements

Do not hyphenate unit modifiers that are chemical names.

- acetic anhydride concentration
- amino acid level
- barium sulfate precipitate
- sodium hydroxide solution
Hyphenate unit modifiers made up of a single letter or number and a noun or adjective.

- $\alpha$-helix structure
- $^{13}$C-enriched proteins
- $^{14}$C-labeling patterns
- d-configuration settings
- $\gamma$-ray spectrometer
- 1-isomer profile
- O-ring suppliers
- $\pi$-electron system
- 3-position substitution
- s-orbital diagrams
- t-test analysis
- U-band transmitter
- x-axis labels
- X-band radar

Do not hyphenate unit modifiers if one of the words is a proper name.

- Fourier transform technique
- Lewis acid catalysis
- Schiff base measurement

Hyphenate unit modifiers that contain spelled-out numbers.

- five-coordinate complex
- one-electron transfer
- seven-membered ring
- three-dimensional model
- three-neck flask
- three-stage sampler
- two-compartment model
- two-phase system

Hyphenate unit modifiers that contain a present or past participle.

- air-equilibrated samples
- English-speaking colleagues
- fluorescence-quenching solution
- hydrogen-bonding group
- immobilized-phase method
- ion-promoted reaction
- laser-induced species
- methyl-substituted intermediate
- photon-induced conversion
- rate-limiting step
- research-related discussion
- steam-distilled sample

**CAUTION** Watch for cases where the participle forms a unit with the noun that follows: for example, “ligand binding site” should not be hyphenated.

Hyphenate unit modifiers of three or more words.

- head-to-head placement
- high-molecular-weight compound
- nine-membered-ring species
- out-of-plane distance
- root-mean-square analysis
- signal-to-noise ratio
- tried-and-true approach
- voltage-to-frequency converter

Hyphenate unit modifiers containing three words when similar two-word modifiers are hyphenated.

- acid-catalyzed reaction
- general-acid-catalyzed reaction
- metal-promoted reaction
- transition-metal-promoted reaction
**Exception** Do not hyphenate unit modifiers containing three or more words, even if similar two-word modifiers are hyphenated, when doing so would break other rules. For example, do not hyphenate unit modifiers if one of the words is a proper name. Do not hyphenate unit modifiers that are two-word chemical names.

- acid-catalyzed reactions (*but* Lewis acid catalyzed reactions)
- copper-to-iron ratio (*but* sodium chloride to iron ratio)

➤ Hyphenate unit modifiers used as predicate adjectives. (*Predicate adjectives* are usually used with the verb “to be”; they are adjectives that modify the subject but come after the verb.) Usually, only unit modifiers that consist of nouns and adjectives or nouns and participles can be used as predicate adjectives.

- All compounds were light-sensitive and were stored in the dark.
- In these cluster reactions, dehydrogenation is size-dependent.
- The antibody is species-specific.
- The complex is square-planar.
- The movie was thought-provoking.
- The reaction is first-order.

➤ Hyphenate phrases also containing en dashes (see pp 124–126) when they are used as unit modifiers.

- alkyl–heavy-metal complexes
- high-spin–low-spin transition
- metal–metal-bonded complexes
- Michaelis–Menten-like kinetics
- retro-Diels–Alder reaction
- transition-metal–chalcogen complexes

➤ Hyphenate phrases containing parenthetical expressions when they are used as unit modifiers.

- element (silicon or tin)-centered radicals

### Capitalization

**In Text**

Generally, in text keep all words lowercase, including chemical names and terms, except proper nouns and adjectives. However, there are many exceptions.

➤ Capitalize the words “figure”, “table”, “chart”, and “scheme” only when they refer to a specific numbered item.

- Chart 4
- Figure 1
- Schemes 4–7
- Table II
Do not capitalize the “r” in “X-ray” at the beginning of a sentence or in a title.

Capitalize parts of a book when they refer to a specific titled and numbered part.

Appendix I
Chapter 3
Section 4.2

But
the appendix
the chapter
the contents
the preface

Capitalize only the name of an eponym, not the accompanying noun.

Avogadro’s number
Boltzmann constant
Einstein’s theory
Graham’s law
Hodgkin’s disease

Lewis acid
nuclear Overhauser effects
Raman spectroscopy
Schiff base

EXCEPTIONS
Nobel Peace Prize
Nobel Prize

Capitalize adjectives formed from proper names.

Boolean Einsteinian Laplacian
Cartesian Freudian Lorentzian
Copernican Gaussian Mendelian
Coulombic Hamiltonian Newtonian
Darwinian

Capitalize the first word after a colon if the colon introduces more than one complete sentence, a quotation, or a formal statement.

Chemists find enzymes attractive as potentially useful synthetic tools for many reasons: Enzymes catalyze reactions with high regio- and stereoselectivity. They cause tremendous rate accelerations under mild reaction conditions. They reduce the need for protecting groups and give enantiomerically pure products.

An emulsion is a thermodynamically unstable system: it has a tendency to separate into two phases.

Two types of asymmetric reactions were conducted: synthesis of styrene oxide and reduction of olefinic ketones.

The editor wishes to make the following point: No papers will receive preferential treatment on the basis of artwork.
Do not capitalize lowercase chemical descriptors hyphenated to chemical names when they are at the beginning of a sentence.

* cis*-4-Chloro-3-buten-2-one was obtained in 74% yield.
* o*-Dichlorobenzene was the solvent.

When the first word of a sentence is a roman chemical descriptor that is not part of a chemical name, capitalize it.

* Cis and trans isomers are used in pharmaceuticals and agrochemicals.*
* Erythro diols were obtained in good yield.*
* Syn hydroxylation of cycloalkenes was attempted.*
* Trans hydroxyl groups are oxidized biochemically.*

Do not capitalize chemical names or nonproprietary drug names unless they are at the beginning of a sentence or are in a title or heading. In such cases, capitalize the first letter of the English word, not the locant, stereoisomer descriptor, or positional prefix. (See Chapter 12, “Names and Numbers for Chemical Compounds”.)

Some reaction names are preceded by element symbols; they may be used as nouns or adjectives. When they are the first word of a sentence or appear in titles and headings, the first letter of the word is capitalized.

* N-Oxidation of the starting compounds yielded compounds 3–10.*
* N-Benzoylated amines undergo hydroxylation when incubated with yeast.*
* Preparation of S-Methylated Derivatives*
* O-Substituted Structural and Functional Analogues*

When a sentence begins with a symbol that is not hyphenated to the following word, the word is not capitalized.

* \( \pi \)-Electron contributions are evident.*
* \( \pi \) electrons make significant contributions in this system.*
* \( \sigma \) values were calculated from eq 3.*

Always capitalize kingdom, phylum, class, order, family, and genus taxonomic names, as well as names of cultivars. Subclassifications follow the same presentation as the main category.

* Animalia, Planta (kingdom)*
* Chordata (phylum)*
* Vertebrata (subphylum)*
* Mammalia, Reptilia (class)*
* Primates, Testudines (order)*
The ACS Style Guide

Hominidae, Apiaceae (family)
_Homo, Drosophila_ (genus)
*Lycopersicon esculentum* Mill. cv. Jennita (cultivar)

Use lowercase for species, subspecies, and varieties, even in titles.

_Escherichia coli_
_Achromobacter haemolyticus_ subsp. _alcaligenes_
_Zea mays_ var. _rugosa_ (variety)

Three New Dihydroisocoumarins from the Greek Endemic Species _Scorzonera cretica_

Do not capitalize the abbreviation for species, singular or plural (sp. or spp., respectively), subspecies (subsp.), variety (var.), or cultivar (cv.).

_Salmonella_ sp.
_Polygonum_ spp.
_Petroselinum crispum_ Mill. subsp. _tuberosum_
_Zea mays_ var. _rugosa_
*Lycopersicon esculentum* Mill. cv. Jennita

Do not capitalize genus names used as common nouns except at the beginning of a sentence or in a title or heading.

bacillus
gorilla, a member of the genus _Gorilla_
hippopotamus, a member of the genus _Hippopotamus_
klebsiella
pseudomonad, a member of the genus _Pseudomonas_
streptococcus

Do not capitalize the adjectival or plural form of a genus name unless it is at the beginning of a sentence or in a title or heading.

bacilli
pneumococcal
streptococcal

In text, do not capitalize polymer names that contain the names of the polymerizing species in parentheses following the prefix “poly”. At the beginning of a sentence, capitalize only the “P” in “poly”.

Poly(vinyl chloride) is a less useful polymer than poly(ethylene glycol).

Capitalize trademarks; use them as adjectives with the appropriate nouns.

Ficoll
Novocain (but novocaine)
Plexiglas (but plexiglass)

Pyrex
Sephadex
Styrofoam

Teflon
Triton
Tween
Do not capitalize the word “model” with a number or code.

- $\gamma$ counter (Beckman model 5500B)
- mass spectrometer (PerkinElmer model 240C)
- multichannel spectrometer (Otsuka model MCPD-1000)
- spectrometer (Varian model XL-200)
- Waters model 660 gradient controller

Do not capitalize the common names of equipment.

- dynamic mechanical analyzer
- electron-diffraction chamber
- flame-ionization detector
- gas chromatograph
- mass spectrometer
- mercury lamp
- spectrophotometer
- temperature controller unit

Use only an initial capital letter, not all capitals, for company names that are not acronyms, because company names are not trademarks and are not protected by law.

- Valspar Corporation
- Xerox Corporation

But

- EMD Chemicals Inc.
- IBM Corporation

Capitalize the names of specific organizations or entities, including ACS local sections, committees, and governing bodies, but not the general terms for them.

- ACS Board of Directors
- ACS Committee on Analytical Reagents
- ACS Division of Fuel Chemistry
- American Chemical Society
- Clean Water Act
- Environmental Protection Agency
- the Milwaukee Section
- University of Michigan
- the board
- an ACS committee
- the division
- the society
- the act
- the agency
- a local section
- the university

Capitalize the names of specific titles when they appear with a person’s name, but not the general terms for them.

- the professor
- the general
- the mayor
- Professor Perry Key
- General James Shore
- Mayor Ralph Estes
- Walter Baldwin, Professor of Chemistry
The well-known professor Perry Key will give a tutorial.
James Shore, a general in the U.S. Army, will teach a graduate course.
Our speaker will be the retired general James Shore.
Isaac Bickford is an assistant professor.
Ralph Estes is the mayor of a small town in upstate New York.

Capitalize the names of special events but not the general terms for them.

229th ACS National Meeting
39th ACS Western Regional Meeting
79th ACS Colloid and Surface Science Symposium
the regional meeting
the spring national meeting
the symposium

Capitalize sections of the country but not the corresponding adjectives.

the Midwest, but midwestern
the Northeast, but northeastern

Do not capitalize the names of the four seasons: summer, fall, autumn, winter, spring.

Capitalize Earth, Sun, and Moon only when used in an astronomical sense.

Venus and Mars are the closest planets to Earth.
The Earth rotates on its axis and revolves around the Sun.
The Moon is the only body that orbits the Earth.

But

Water bodies on the earth’s surface contain a variety of chromophoric substances.
Pollution occurs to some extent everywhere on earth.
The sun is the primary source of radiation that can cause chemical transformations.
The next full moon will be on Thursday.

In Titles and Headings

These guidelines apply to titles and headings at all levels; that is, they apply to subtitles and subheadings. They also apply to table, scheme, and chart titles.

In titles and headings that are typeset in capital and lowercase letters, capitalize the main words, which are nouns, pronouns, verbs, adjectives, adverbs, and
subordinating conjunctions, regardless of the number of letters. Do not capitalize coordinating conjunctions (“and”, “but”, “or”, “nor”, “yet”, “so”), articles (“a”, “an”, “the”), or prepositions. Do capitalize the “to” in infinitives. Do capitalize the first and last words of a title or heading, regardless of part of speech, unless the word is mandated to be lowercase (e.g., pH, d Orbital).

Changes in the Electronic Properties of a Molecule When It Is Wired into a Circuit
Derivatives from a Chiral Borane–Amine Adduct
In Situ Nutrient Analyzer
In Vitro and in Vivo Antiestrogenic Effects of Polycyclic Musks in Zebrafish
Nickel-Catalyzed Addition of Grignard Reagents: Ring-Opening Reactions with Nucleophiles
Phosphonolipids with and without Purified Hydrophobic Lung Surfactant Proteins
Properties of Organometallic Fragments in the Gas Phase
Reactions of Catalyst Precursors with Hydrogen and Deuterium
Scope of the Investigations: The First Phase
The Computer as a Tool To Improve Chemistry Teaching
Vibrations in Situ

**EXCEPTION 1** In titles and headings, capitalize small words that are parts of phrasal verbs.

- Break Down
- Set Up
- Build Up
- Slow Down
- Set Off
- Wear Out

**EXCEPTION 2** In titles and headings, capitalize small words that are parts of phrasal adjectives.

- End-On Bonding
- In-Plane Atoms
- Side-On Bonding

(But Out-of-Plane Vibrations [only the first preposition is capitalized])

➤ In titles and headings, capitalize “as” when it is used as a subordinating conjunction but not when it is used as a preposition.

Alumina as a Catalyst Support
Kinetics of Cyanocobalamin As Determined by Binding Capacity

➤ Do not capitalize the “r” in “X-ray” in titles and headings. Do capitalize the “r” in “γ ray” and the “p” in “α particle” and “β particle” in titles and headings.
Do not capitalize lowercase chemical descriptors in titles and headings, but do capitalize the first letter of the English word.

Reaction of trans-4-(Phenylsulfonyl)-3-buten-2-one

When abbreviated units are acceptable in titles and headings, do not capitalize those that are ordinarily lowercase.

Analysis of Milligram Amounts
Determination of N-Nitrosodimethylamine at Concentrations <7 ng/L

Always capitalize genus names, but never capitalize species names, in titles and headings.

Active-Site Nucleophile of Bacillus circulans Xylanase
Novel Metabolites of Siphonaria pectinata

In titles and headings, capitalize all main words in a unit modifier.

Base-Catalyzed Cyclization
Cross-Linked Polymer
Deuterium-Labeling Experiment
High-Temperature System
Non-Hydrogen-Bonding Molecules
Thyrotropin-Releasing Hormone

In titles and headings, capitalize each component of compound words if the component would be capitalized when standing alone.

Cross-Link
Half-Life
Quasi-Elastic

Do not capitalize hyphenated suffixes.

Synthesis of Cubane-like Clusters

In titles and headings, capitalize only the first letter (“P”) of polymer names that contain the names of the polymerizing species in parentheses following the prefix “poly”.

IR Spectroscopic Analysis of Poly(1H,1H-fluoroalkyl α-fluoroacrylate)
Light-Scattering Studies of Poly(ethylene-co-butylene)
New Uses for Poly(ethylene terephthalate)
Polystyrene-block-poly(2-cinnamoylethyl methacrylate) Adsorption
Reactions of Poly(methyl methacrylate)
Synthesis and Characterization of Poly(isobutylene-b-methyl vinyl ether)
Capitalize only the first letter in a chemical name containing complex substituents in parentheses or brackets.

2-[3-[2-[2S]-2-Cyano-1-pyrrolidinyl]-2-oxoethylamino]-3-methyl-1-oxobutyl]-1,2,3,4-tetrahydroisoquinoline: A Potent, Selective, and Orally Bioavailable Dipeptide-Derived Inhibitor of Dipeptidyl Peptidase IV

Preparations of (Methyl isocyanide)iron Compounds

Structures of Tetrakis(methyl isocyanide)iron Complexes

Capitalize parenthetical phrases in titles and headings as if they were not parenthetical.

Versatile Organic (Fullerene)–Inorganic (CdTe Nanoparticle) Nanoensembles

Surnames

Capitalization

Although a current trend is to lowercase the surnames of persons when these names are used as modifiers and have become very familiar, many are still capitalized. The following is a list (by no means complete) of names that should be capitalized.

Avogadro  Claisen  Markovnikov
Beckmann  Dewar benzene, flask  Mössbauer
Beilstein  Dreiding  Petri
Boltzmann  Erlenmeyer  Poiseuille
Bragg  Gram  Poisson
Bronsted  Kekulé  Priestley
Büchner  Kjeldahl  Scatchard
Bunsen  Mahalanobis  VandenHeuvel

EXCEPTIONS

de Broglie
van der Waals
van’t Hoff

Surnames that are used as units of measure are lowercase.

ampere  einstein  hertz  poise
angstrom  faraday  joule  siemens
coulomb  gauss  kelvin  sievert
curie  gilbert  langmuir  stokes
dalton  gray  newton  tesla
darcy  hartree  ohm  watt
dehbye  henry  pascal  weber
In the temperature–current curves, temperature is given in kelvins and current is shown in amperes.

NMR coupling constants are reported in hertz.

**Hyphenation**

- Hyphenation of double surnames is discussed on p 139.

- Hyphenate prefixes and suffixes to proper names as nouns and adjectives, and retain the capital letter.
  
  anti-Markovnikov  non-Gaussian
  hetero-Diels–Alder  non-Newtonian
  Kennedy-like  oxy-Cope
  Michaelis–Menten-like  retro-Diels–Alder
  non-Coulombic

**Foreign Surnames**

Some foreign surnames follow a format different from the American system. The Chinese use their surnames first, followed by their given names. For example, Sun Yat-sen’s surname is Sun. However, the problem of identifying surnames extends to many other cultures. This multiplicity of usage can create problems in bibliographic indexes and in reference citations. A reference citation in a bibliography should always list the surname first, followed by given name or initials. In a byline, the author names should be presented in standard American format (given names first and surnames last) to ensure consistency of citation practice. If a footnote would clarify the situation or eliminate any perceived confusion, use a footnote.

In most cultures, the surname is the family name, but it may not be the formal name, that is, the name or shortest string of names that are properly used following a title (Mr., Dr., Professor, etc.). Presented here are some cases in which different customs are used for the order of surnames, given names, and formal names. This list is by no means complete, but at least it will help you to be aware of these differences.

**Arabic** Often many names; the position of the surname is highly variable. The formal name often consists of two or three names, including articles that can be joined. Examples: Ibn Saud, Abd al-Qadir.

**Chinese** Two or three names; the surname is first. Examples: Chiang Kai-shek is Dr. Chiang; Chou En-lai is Dr. Chou.

**Hebrew** Two or three names; the surname is the last one or two and is the formal name. Examples: David Ben-Gurion is Dr. Ben-Gurion; Moshe Bar-Even is Dr. Bar-Even.
HUNGARIAN  Two names; the surname is first, and it is the formal name. However, the second name is accepted as formal internationally.

JAPANESE  Two names; the surname is the formal name. The surname is first in Japanese. However, when the names are translated into non-Asian languages, surnames appear last. Example: Taro Yamada is Dr. Yamada.

KOREAN  Usually three names; the surname is first and is the formal name. In North Korean names, all three parts start with a capital letter. Examples: Kim Il Sung is Dr. Kim. In South Korean names, the two parts of the given name are hyphenated, and the second part is lowercase. Example: Kim Young-sum is Dr. Kim.

SPANISH  Frequently three or more names; the last two are surnames, sometimes connected by “y”. The second surname is often dropped or abbreviated. The formal name begins with the first surname and includes the second surname only in very formal usage. Example: Juan Perez Avelar is Dr. Perez or Dr. Perez Avelar, but never Dr. Avelar. The two surnames may also be hyphenated. Example: Jose Gregorio Angulo-Vivas is Dr. Angulo or Dr. Angulo-Vivas, but never Dr. Vivas.

THAI  Two names; the surname is last, but the formal name is first.

VIETNAMESE  Two or three names; the first is the surname and formal name.

INITIALS  Some foreign names are abbreviated with two-letter initials that reflect transliteration from a non-Latin alphabet: Ch., Kh., Ph., Sh., Th., Ts., Ya., Ye., Yu., and Zh.

Some foreign names are abbreviated with hyphenated initials: C.-C. Yu.

Special Typefaces

Special typefaces help the reader quickly distinguish certain letters, words, or phrases from the rest of the text.

Italic Type

Chapter 11 describes the use of italic type in mathematical material, and Chapters 12 and 13 give guidelines for the use of italic type in chemical names and conventions in chemistry.

➤  Use italic type sparingly to emphasize a word or phrase. Do not use italics for long passages.
Use italic type for a word being defined or for a newly introduced term the first time it appears in text.

In an *outer-sphere transfer*, an electron moves from reductant to oxidant with no chemical alteration of the primary coordination spheres.

We call these materials *microcapsules*.

Use italic type for the titles and abbreviations of periodicals, books, and newspapers. If “the” is the first word of the title, italicize and capitalize it.

An article on a promising cholesterol biosynthesis inhibitor appeared in *The Journal of Organic Chemistry* this month.

*Enough for One Lifetime* is the biography of Wallace Carothers.

I read three articles on that new chiral compound in the *Journal of the American Chemical Society*.

*The Washington Post* did a feature story on the president’s daughter.

Do not use italic type for common Latin terms and abbreviations.

<table>
<thead>
<tr>
<th>a priori</th>
<th>e.g.</th>
<th>in vitro</th>
</tr>
</thead>
<tbody>
<tr>
<td>ab initio</td>
<td>et al.</td>
<td>in vivo</td>
</tr>
<tr>
<td>ad hoc</td>
<td>etc.</td>
<td>status quo</td>
</tr>
<tr>
<td>ca.</td>
<td>i.e.</td>
<td>vs</td>
</tr>
<tr>
<td>de novo</td>
<td>in situ</td>
<td></td>
</tr>
</tbody>
</table>

Use italic type for genus, species, subspecies, and variety names of all animals, plants, and microorganisms, but not when these names are used as singular or plural common nouns or when they are adjectival.

a bacterium of the genus *Salmonella*

*Bacillus coagulans* and *Bacillus dysenteriae* are two species of bacilli.

*Staphylococcus aureus* is the bacterium that causes staphylococcal infection.

*Streptococcus pneumoniae* (genus and species)

The red rhododendron, *Rhododendron arboreum*, needs bright sun.

*Achromobacter haemolyticus* subsp. *alcaligenes* (subspecies)

*Zea mays* var. *rugosa* (variety)

Use italic type for genotypes (representations of genes) and roman type for phenotypes (representations of proteins).

The *vanA* gene that encodes one such inducible resistance protein is designated VanA.

*E. coli* DH5α Δ(lacZYA–argF)U169 deoR recA1 endA1 hsdR17(rK+ mK+) supE44 λ− thi–1 gyrA96 relA1 F' proAB+ lacIqZ Δ M15 ssf::Tn5 [Km+]
Names of restriction endonucleases should follow the typeface conventions of the names from which they were derived: use italic type for the three-letter portion derived from the genus and species name; use roman type for additional strain designators (letters and/or arabic numerals) and for the roman numeral identifiers.

\begin{tabular}{ccc}
BamHI & HaeIII & SmaI \\
EcoRI & HindIII & XhoI \\
HaeII & SaeI & Sau3AI \\
\end{tabular}

**Exception** Use roman type for abbreviations of general enzyme types.

- Exo III for exonuclease III
- Pol α for DNA polymerase α
- Topo II for topoisomerase II

- Do not use italic type for “pH”; “p” is always lowercase, and “H” is always capitalized.

- Do not use italic type for M (molar) or N (normal). Do use italic type for \( m \) (molal).

**Greek Letters**

- Use Greek letters, not the spelled-out words, for chemical and physical terms. Do not italicize Greek letters.
  - \( \alpha \) helix (not alpha helix)
  - \( \beta \) particle (not beta particle)
  - \( \beta \) sheet (not beta sheet)
  - \( \gamma \) radiation (not gamma radiation)
  - NFκB (nuclear factor κB) (not NF kappa B)

**Exceptions**

- delta opioid receptor
- mu opioid receptor

**Computer-Related Usage**

- Capitalize the first letter of the names of computer languages.

\begin{tabular}{ccc}
AP & Fortran & Perl \\
Basic & Java & Python \\
Cobol & Logo & Smalltalk \\
Eiffel & Pascal & \\
\end{tabular}
Capitalize the first letter of the names of programs, and follow the manufacturer’s or creator’s usage within the name.

Acrobat
Alchemy
ChemDraw
ChemIntosh
ChemPlus
EasyPlot
EndNote
FileMaker Pro
Freehand
HyperChem
ISIS/Draw
KaleidaGraph
LaTeX
Mathematica
MathType
Microsoft Excel
Microsoft PowerPoint
Microsoft Word
Molecular Presentation Graphics
MULTAN78
Oracle
Photoshop
ProCite
SigmaPlot
SIM4A
Symphony
TK Solver
Un-Plot-It
UniVersions
WordPerfect

Use lowercase letters for the spelled-out forms of protocols, except as the first word of a sentence and in titles and headings.

network news-transfer protocol (NNTP)

Appendix 10-1 contains a list of some common computer and Internet terms.

**Uniform Resource Locators**

A typical uniform resource locator (URL), which is an address on the World Wide Web, takes the following forms:

http://www.domain.zone

http://www.domain.zone/name1/~name2/

http://domain.zone/name1/~name2/name3.html

The number of names varies. For example,

http://www.chemistry.org

http://nobelprize.org/chemistry/index.html

These examples are short, but URLs can be quite long, and in narrative text they often will need to be broken at the end of a line. If the URL does not fit on one line, it can be broken according to the following guidelines:

➤ Break after an ampersand, a slash, or a period, but keep two slashes together.

➤ Do not add a hyphen to the end of the line.

➤ Do not break after a hyphen to avoid confusion as to the hyphen’s purpose.
E-Mail Addresses

A typical e-mail address usually takes one of these forms:

- personname@companyname.zone
- initial.surname@companyname.zone
- surname.initial@companyname.zone

All kinds of variations on the person’s name and initials are possible, and besides the underscore, other types of punctuation are used. Long names are often truncated.

➤ Break e-mail addresses in text after the @ or a period. Do not insert a hyphen or any other character.

Chapter 14, “References”, presents the editorial style for electronic sources listed in reference lists and bibliographies.

Trademarks

A trademark is an adjective that describes a material or product (e.g., Teflon resin, Kleenex tissue). The term “brand name” is a synonym for trademark. In ACS publications, do not use the trademark symbols ™ and ® or the service mark symbol SM. They are not necessary to ensure legal protection for the trademark.

➤ Capitalize trademarks; use them as adjectives with the appropriate nouns. Do not use them in titles.

- Ficoll
- Novocain (*but* novocaine)
- Plexiglas (*but* plexiglass)
- Pyrex
- Sephadex
- Styrofoam
- Teflon
- Triton
- Tween

➤ In general, however, use generic names rather than trade names.

- cross-linked dextran polymer beads (*not* Sephadex)
- diatomaceous earth (*not* Celite)
- 4,4’-isopropylidenediphenol (*not* Bisphenol A)
- 2-methoxyethanol (*not* Methyl Cellosolve)
- mineral oil (*not* Nujol)
- paclitaxel (*not* Taxol)
- petroleum jelly (*not* Vaseline)
- photocopy (*not* Xerox)
- poly(ethylene glycol) (*not* Carbowax)
- tensile testing machine (*not* Instron tester)

➤ Use trademarks as adjectives only, never as nouns or verbs. Because trademarks are adjectives, they do not have plural forms.
Abbreviations and Acronyms

An abbreviation is a short form of a word; often the individual letters are pronounced. In an acronym, the letters always form a pronounceable word. ACS is an abbreviation; CASSI is an acronym.

A list of ACS-recommended abbreviations, acronyms, and symbols is given in Appendix 10-2. Check the list to find an abbreviation. If no abbreviation is listed for the term you are using, you may devise an abbreviation provided that (1) it is not identical to an abbreviation of a unit of measure, (2) it will not be confused with the symbol of an element or a group, (3) it does not hamper the reader’s understanding, and (4) you do not use the same abbreviation for more than one spelled-out form.

If a very long name or term is repeated many times throughout a paper, an abbreviation is warranted. Place the abbreviation in parentheses following the spelled-out form the first time it appears in the text. If it is used in the abstract, define it in the abstract and again in the text. After defining the abbreviation in the text, you may use it throughout the paper.

Exceptions The following list shows abbreviations that never need to be defined. Refer to Appendix 10-2 for all other abbreviations.

- a.m. before noon (Latin ante meridiem)
- anal. analysis
- at. wt atomic weight
- bp boiling point
- ca. about (Latin circa)
- cf. compare (Latin confer)
- CP chemically pure
- DNA deoxyribonucleic acid
- e.g. for example (Latin exempli gratia)
- ed., eds. edition, editions
- Ed., Eds. Editor, Editors
- eq(s) equation(s) [with number(s)]
- equiv equivalent(s) [with number(s)]
- equiv wt equivalent weight
- et al. and others (Latin et alii)
- etc. and so forth (Latin et cetera)
- fp freezing point
- GLC gas–liquid chromatography
- i.d. inside diameter
- i.e. that is (Latin id est)
- in. inch, inches
- IR infrared
- m molal
- M molar
Avoid abbreviations in the title of a paper.

For some, but not all, abbreviations, case is important; that is, if they are capitalized, they must never be made lowercase; if they are lowercase, they must never be capitalized. This guideline applies to abbreviations that would lose their meanings or change meanings if their forms were changed, such as units of measure (e.g., mg cannot be changed to Mg, min cannot be changed to Min), mathematical symbols (e.g., pH cannot be changed to PH or ph), and chemical symbols (e.g., o for ortho cannot be changed to O).

However, if the meaning would not be affected, some abbreviations can be capitalized at the beginning of a sentence and in titles and headings, especially if they are so common that they are more like words than abbreviations. For example, you could use “e-mail” in text and “E-mail” at the beginning of a sentence.

Symbols for the chemical elements are not treated as abbreviations. They need not be defined, and they are typeset in roman type. (See Table 13-1 on p 270 f.)
Abbreviate units of measure and do not define them when they follow a number. Without a number, spell them out.

\[ 9 \text{ V/s or } 9 \text{ V} \cdot \text{s}^{-1} \text{ (but measured in volts per second) } \]

For exceptions, see p 225.

Abbreviations that are common to a specific field may be permitted without identification in books and journals in that field only, at the discretion of the editor.

For genus and species names, spell out the full genus name in the title, in the abstract, and the first time it appears in text. Abbreviate it thereafter with the same species name, but spell it out again with each different species name. Form the abbreviation with the initial of the genus name. If the paper contains more than one genus name that starts with the same initial letter, devise abbreviations that distinguish them. Use italic type for all names and abbreviations.

<table>
<thead>
<tr>
<th>FIRST TIME</th>
<th>SUBSEQUENTLY</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>Bacillus stearothermophilus</em></td>
<td><em>B. stearothermophilus</em></td>
</tr>
<tr>
<td><em>Bacillus subtilis</em></td>
<td><em>B. subtilis</em></td>
</tr>
<tr>
<td><em>Escherichia coli</em></td>
<td><em>E. coli</em></td>
</tr>
<tr>
<td><em>Salmonella typhimurium</em></td>
<td><em>S. typhimurium</em></td>
</tr>
<tr>
<td><em>Staphylococcus aureus</em></td>
<td><em>Staph. aureus</em></td>
</tr>
</tbody>
</table>

Use “e.g.,” “i.e.,” “vs.”, and “etc.” only in figure captions, in tables, and in parentheses in text. Elsewhere, spell out “for example”, “that is”, “versus”, and “and so forth”.

Do not confuse abbreviations and mathematical symbols. An abbreviation is usually two or more letters; a mathematical symbol should generally be only one letter, possibly with a subscript or superscript. An abbreviation may be used in narrative text but seldom appears in equations; a mathematical symbol is preferred in equations and may also be used in text. For example, in text with no equations, \( P_E \) may be used for potential energy, but in mathematical text and equations, \( E_p \) is preferred. Abbreviations are typeset in roman type; most mathematical symbols are typeset in italic type.

In text, spell out all months with or without a specific day.

On August 3, 1996, we completed the second phase of the experiment.

The final results will be available in January 1997.

Use the following abbreviations (with no periods) or spelled-out forms for months with a day or with a day and year in footnotes, tables, figure captions, bibliographies, and lists of literature cited.
Use the abbreviations U.S. and U.K. as adjectives only; spell out United States and United Kingdom as the noun forms in text. Either United Kingdom or U.K. may be used in addresses.

- U.K. educational system
- educational system in the United Kingdom
- U.S. science policy
- chemical industry in the United States

Form the plurals of multiletter, all-capital abbreviations and abbreviations ending in a capital letter by adding a lowercase “s” only, with no apostrophe.

- HOMOs
- JPEGs
- PAHs
- PCBs
- PCs
- pHs

To avoid ambiguity or poor appearance, add an apostrophe and a lowercase “s” to form the plurals of lowercase abbreviations, single-capital-letter abbreviations, abbreviations ending in a subscript or superscript, and abbreviations ending in an italic letter.

- cmc’s
- O’s (or oxygens; Os is the symbol for osmium)
- pK’s
- pK̄’s
- $T_g$’s

Use two-letter abbreviations for U.S. state and territory names and the District of Columbia and for Canadian province and territory names on all letters going through the U.S. Postal Service and most express delivery services. Use them after the name of a city in text, footnotes, and references.

**U.S. STATES, TERRITORIES, AND THE DISTRICT OF COLUMBIA**

<table>
<thead>
<tr>
<th>Alabama</th>
<th>AL</th>
<th>Colorado</th>
<th>CO</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alaska</td>
<td>AK</td>
<td>Connecticut</td>
<td>CT</td>
</tr>
<tr>
<td>American Samoa</td>
<td>AS</td>
<td>Delaware</td>
<td>DE</td>
</tr>
<tr>
<td>Arizona</td>
<td>AZ</td>
<td>District of Columbia</td>
<td>DC</td>
</tr>
<tr>
<td>Arkansas</td>
<td>AR</td>
<td>Federated States of Micronesia</td>
<td>FM</td>
</tr>
<tr>
<td>California</td>
<td>CA</td>
<td>Florida</td>
<td>FL</td>
</tr>
<tr>
<td>State/Province/Region</td>
<td>Abbreviation</td>
<td>City/State/Region</td>
<td></td>
</tr>
<tr>
<td>-------------------------------------------</td>
<td>--------------</td>
<td>------------------------------------</td>
<td></td>
</tr>
<tr>
<td>Georgia</td>
<td>GA</td>
<td>New York</td>
<td></td>
</tr>
<tr>
<td>Guam</td>
<td>GU</td>
<td>North Carolina</td>
<td></td>
</tr>
<tr>
<td>Hawaii</td>
<td>HI</td>
<td>North Dakota</td>
<td></td>
</tr>
<tr>
<td>Idaho</td>
<td>ID</td>
<td>Northern Mariana Islands</td>
<td></td>
</tr>
<tr>
<td>Illinois</td>
<td>IL</td>
<td>Ohio</td>
<td></td>
</tr>
<tr>
<td>Indiana</td>
<td>IN</td>
<td>Oklahoma</td>
<td></td>
</tr>
<tr>
<td>Iowa</td>
<td>IA</td>
<td>Oregon</td>
<td></td>
</tr>
<tr>
<td>Kansas</td>
<td>KS</td>
<td>Palau</td>
<td></td>
</tr>
<tr>
<td>Kentucky</td>
<td>KY</td>
<td>Pennsylvania</td>
<td></td>
</tr>
<tr>
<td>Louisiana</td>
<td>LA</td>
<td>Puerto Rico</td>
<td></td>
</tr>
<tr>
<td>Maine</td>
<td>ME</td>
<td>Rhode Island</td>
<td></td>
</tr>
<tr>
<td>Marshall Islands</td>
<td>MH</td>
<td>South Carolina</td>
<td></td>
</tr>
<tr>
<td>Maryland</td>
<td>MD</td>
<td>South Dakota</td>
<td></td>
</tr>
<tr>
<td>Massachusetts</td>
<td>MA</td>
<td>Tennessee</td>
<td></td>
</tr>
<tr>
<td>Michigan</td>
<td>MI</td>
<td>Texas</td>
<td></td>
</tr>
<tr>
<td>Minnesota</td>
<td>MN</td>
<td>Utah</td>
<td></td>
</tr>
<tr>
<td>Mississippi</td>
<td>MS</td>
<td>Vermont</td>
<td></td>
</tr>
<tr>
<td>Missouri</td>
<td>MO</td>
<td>Virgin Islands</td>
<td></td>
</tr>
<tr>
<td>Montana</td>
<td>MT</td>
<td>Virginia</td>
<td></td>
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<td>CANADIAN PROVINCES AND TERRITORIES</td>
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<td>Ontario</td>
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<td>MB</td>
<td>Prince Edward Island</td>
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<td>NB</td>
<td>Quebec</td>
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<tr>
<td>Newfoundland and Labrador</td>
<td>NL</td>
<td>Saskatchewan</td>
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<td>Northwest Territories</td>
<td>NT</td>
<td>Yukon Territory</td>
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</tr>
<tr>
<td>Nova Scotia</td>
<td>NS</td>
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</tr>
</tbody>
</table>

➤ Spell out and capitalize “company” and “corporation” as part of company names when they appear in an author’s affiliation. Abbreviate them elsewhere in text. After the first mention, drop Co. and Corp. and use only the company name.
APPENDIX 10-1

Computer and Internet Terms

This appendix lists the spelling, capitalization, and abbreviations of some common computer and Internet terms. This list is not intended to be exclusive. Alternative choices, in many cases, are acceptable. Proscribed usages are specifically indicated.

An excellent source for definitions of these terms may be found at http://www.google.com/. In the search statement, use the syntax “define:xyz” where xyz is the term for which a definition is sought.

active matrix  bounce (e-mail)
ADSL (asymmetric digital subscriber line)  bps (bits per second)
AI (artificial intelligence)  broadband
anonymous FTP  browser
applet  bulletin board
application  byte
archive  C (programming language)
ASCII (American Standard Code for  C++ (programming language)
Information Interchange)  cache
ASP (application service provider)  CAD (computer-assisted design)
asynchronous  CAD/CAM (computer-assisted design
AVI (audio video interleaved) and manufacturing)
back up (verb)  CCD (charge-coupled device)
backup (noun, adjective)  CD (compact disc)
bandwidth  CD key
Base 64  CD-R (compact disc read-only)
batch processing  CD-ROM (compact disc with read-only
baud memory)
baud rate  CD-RW (compact disc read-write)
BBS (bulletin board system)  CDMA (code division multiple access)
BinHex (binary hexadecimal)  CGI (common gateway interface)
BIOS (basic input/output system)  CGM (computer graphics metafile)
bit  CIF (crystallographic information file)
bitmap  codec
Bitnet (Because It’s There NETwork)  compact disc (CD)
bitstream  compiler
blog, blogger  CPU (central processing unit)
bookmark  CRT (cathode ray tube)
boot
CSS (cascading style sheet)
cursor
CVC (color video controller)
cyberspace
daemon
data domain
data log
data parse, data parsing
data processing
data set
database
DBMS (database management system)
debug (verb)
default
defragment
desktop
DHCP (dynamic host configuration protocol)
DHTML (dynamic hypertext markup language)
dialog box
digital signal
directory
disc (compact disc only)
disk (floppy or hard disk)
disk drive
disk space
diskette
DNS (domain name system or server)
domain name
DOI (digital object identifier)
DOS (disk operating system)
double-click (as verb)
download
dpi (dots per inch)
drag and drop
DSL (digital subscriber line)
DTD (document-type definition)
duplex
DVD (digital video disc)
DVD-R (digital video disc read-only)
DVD-RW (digital video disc read–write)
e-book
e-journal
e-mail (electronic mail)
e-money
e-publish
e-zine (electronic magazine)
EBCDIC (Extended Binary-Coded Decimal Interchange Code)
emoticons
encryption
end user (noun)
EPS (encapsulated PostScript)
Ethernet (but an ethernet)
extranet
FAQ (frequently asked question)
FDDI (fiber distributed data interface)
fiber optics
file compression
file name
filter
finger
Firefox
firewall
FireWire
flash memory
floppy disk
flowchart
format, formatted, formatting
Fortran
FreeNet (but a freenet)
freeware
front end
FTP (file transfer protocol)
gateway
GB (gigabyte, equal to 1024 megabytes; always a space between number and GB)
GDDM (graphical data display manager)
GDI (graphics device interface)
GIF (graphics interchange format)
4GL (fourth-generation language)
glyph
Google
GPIB (general purpose interface bus)
graphic (noun)
graphical interface
graphics (adjective)
graphics conversion
graphics files
graphics terminal emulation
GUI (graphical user interface)

hard disk
hard disk drive
hardware
hardwired
high-level-language compiler
home directory
home page (lowercase, but capitalized when part of a specific name, e.g., ACS Home Page)
hot key
hotline
HTML (hypertext markup language)
HTTP (hypertext transfer protocol)
HTTPS (hypertext transfer protocol secure)
hyperlink
hypermedia
hypertext

IBM-compatible
icon
iconization
iconize
IM (instant messaging)
IMAP (Internet message access protocol)
information superhighway
input
integrated circuit
interdomain conversion
Internet
intranet
I/O (input/output)
IP (Internet protocol)
IP address
IRC (Internet relay chat)
ISDN (integrated services digital network)
ISP (Internet service provider)

Java
Javascript

JDK (Java Development Kit)
joystick
JPEG (Joint Photographic Experts Group)

K (kilobyte, equal to 1024 bytes; always closed up to number; as in 8K or 16K disk drive; kB is preferred)
kB (kilobyte, equal to 1024 bytes; always a space between number and kB)
KB (kilobyte; kB is preferred)
kbps (kilobits per second)
kBps (kilobytes per second)
keyboard
keypad
keystroke
kilobit
kilobyte

LAN (local area network)
laptop
LaTeX (pronounced “lahtek”)
LCD (liquid-crystal display)
Lexis
LexisNexis
list-administration software
list-management software
list owner
list server
Listserv (software)
local area network (LAN)
log in, logging in (verb)
log off, logging off (verb)
log on, logging on (verb)
log out, logging out (verb)
login name
logon name

Macintosh, Macintoshes
macro, macros
mainframe
math coprocessor
MB (megabyte, equal to 1024 kilobytes; always a space between number and MB)
megapixel
meta-list
metadata
microchip
microcomputer, microcomputing
microprocessor
Microsoft Excel
Microsoft PowerPoint
Microsoft Windows
Microsoft Word
MIDI (musical instrument digital interface)
MIME (multipurpose Internet mail extension)
minicomputer
minifloppy disk
modem
monitor (noun)
motherboard
motif
mouse (plural: mouse devices)
Mozilla
MP3 (MPEG audio layer 3)
MPEG (Motion Picture Experts Group)
MS-DOS (Microsoft disk operating system, always hyphenated)
MTA (mail-transfer agent)
MUA (mail-user agent)
multitasking
NCP (network control program)
NCSA (National Center for Supercomputing Applications)
Net (when referring to the Internet; lowercase when referring to any network)
etiquette
netizen
Netscape
netware
network
newsgroup
NIC (Network Information Center)
NNTP (network news transfer protocol)
node, nodes
NREN (National Research and Education Network)
OCR (optical character recognition)
ODBC (open database connectivity)
off-site (always hyphenated)
offline (one word in computer context)
on-site (always hyphenated)
online (one word in computer context)
open source
OS (operating system)
OSX (Macintosh Operating System X)
output
PageMaker
PAM (pulse amplitude modulation)
parallel port
parser
password
path
PC (personal computer)
PCMCIA (Personal Computer Memory Card International Association)
pdb (Protein Data Bank) format
PDF (portable document format)
Perl (programming language)
PHP (personal home page)
PIF (picture interchange format)
pixel
plaintext
plug and play
plug-in
PNG (portable network graphics)
POP (post office protocol)
popup
PostScript
PPP (point-to-point protocol)
primary domain
print queue
programmer, programming
PROM (programmable read-only memory)
protocol
proxy server
PSTN (public switched telephone network)
pull-down (adjective)
QuarkXPress
queue
QuickTime
RAM (random-access memory)
raster, rasterize
RDBMS (relational database management system)
read/write permission
real time (noun)
real-time (unit modifier)
reboot
RFC (request for comments)
rich text
RJE (remote job entry)
ROM (read-only memory)
router
RPG (report program generator)
RSS (rich site summary)
RTF (rich text format)
run time (noun)
run-time (adjective)
Safari
scale up (verb)
scanner
screen dump
script
SCSI (small computer system interface, pronounced “skuzzy”)
search engine
security certificate
serial communication
serial port
server
servlet
set up (verb)
setup (noun)
SGML (standard generalized markup language)
shared user
shareware
shortcut
shut down (verb)
shutdown (noun, adjective)
sign off (verb)
sign-off (noun, adjective)
simplex
SLIP (serial-line Internet protocol)
SMB (server message block)
SMDS (switched multimegabit data service)
smiley (the :) or ☺ symbol
SMTP (simple mail transfer protocol)
SNMP (simple network management protocol)
SOAP (simple object access protocol)
software
source code
spam
spelling checker
spreadsheet
spyware
SQL (structured query language)
SSL (secure sockets layer)
stand-alone (always hyphenated)
start up (verb)
startup (noun)
strikethrough
submenu
SVGA (super video graphics adapter)
systems programs
T-1, T-3
TB (terabyte)
Tcl (programming language, pronounced “tickle”)
TCP (transmission control protocol)
TCP/IP (transmission control protocol/Internet protocol)
telecommute
Telnet
terminal emulation program
terminal server
TeX (pronounced “tek”)
TFT (thin-film transistor)
throughput
TIFF (tagged image file format)
time-sharing (always hyphenated)
TLD (top-level domain)
toolbar
toolbox
trackball
Trojan horse
TTL (transistor–transistor logic)
TTY (teletype)
UDP (user datagram protocol)
UGA (ultra graphics accelerator)
Unicode
Unify
Unix
upload
UPS (uninterruptible power source)
URC (uniform resource characteristic)
URC (uniform resource identifier)
URL (uniform resource locator)
URN (uniform resource name)
USB (universal serial bus)
Usenet
user id, user ids
utility program
uuencode (Unix-to-Unix encoding)
vector, vectorize
VGA (video graphics adapter)
video adapter
Visual Basic
VoIP (voice over Internet protocol)
VPN (virtual private network)
VRML (virtual reality modeling language)
W3C (World Wide Web Consortium)
WAIS (wide-area information service or server)
WAN (wide-area network)
the Web
Web browser
Web page
Web server
Web site
Webmaster
Webzine
Wi-Fi (wireless fidelity)
window (general term, not specific program)
Windows (Microsoft program)
WinZIP
word-processing software
word processor
WordPerfect
wordwrap
workstation
World Wide Web (three words, no hyphens)
World Wide Web Consortium (W3C)
worm
WORM (write once, read many times)
WWW (World Wide Web)
WYSIWYG (what you see is what you get)
Xbase
Xenix
XML (extensible markup language)
ZIP archive
APPENDIX 10-2

Abbreviations, Acronyms, and Symbols

This list is not intended to be exclusive. Alternative choices, in many cases, are acceptable. Proscribed usages are specifically indicated. If no abbreviation is listed for the term you are using, you may devise an abbreviation provided that (1) it is not identical to an abbreviation of a unit of measure, (2) it will not be confused with the symbol of an element or a group, (3) it does not hamper the reader’s understanding, and (4) you do not use the same abbreviation for more than one spelled-out form.

\( \alpha \)  
fine structure constant  
optical rotation  
stereochemical descriptor

\([\alpha]_D^t\)  
specific rotation at temperature \( t \) and wavelength of sodium D line

\([\alpha]_\lambda^t\)  
specific rotation at temperature \( t \) and wavelength \( \lambda \)

\( a \)  
antisymmetric  
are (unit of area, 100 m\(^2\))  
atto (10\(^{-18}\))  
axial [\( use 2(a)\)-methyl in names]

\( a_0 \)  
Bohr radius (0.52917 Å)

\( A \)  
adenosine  
alanine  
ampere  
ring (italic in steroid names)

\( \text{Å} \)  
angstrom

\( A \)  
absorbance [as in \( A = \log(l/T) \)]  
anticlockwise (chirality symbol)  
Helmholtz energy  
mass number

A.D.  
anno Domini

a.m.  
ante meridiem

AAS  
atomic absorption spectroscopy

abs  
absolute

ac  
alternating current

\( ac \)  
anticlinal
<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ac</td>
<td>acetyl</td>
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<tr>
<td>actinum</td>
<td></td>
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<tr>
<td>acac</td>
<td>acetylacetonato (ligand)</td>
</tr>
<tr>
<td>acam</td>
<td>acetamide (ligand)</td>
</tr>
<tr>
<td>AcCh</td>
<td>acetylcholine</td>
</tr>
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<td>AcChE</td>
<td>acetylcholinesterase</td>
</tr>
<tr>
<td>AcO</td>
<td>acetate</td>
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<td>ACTH</td>
<td>adrenocorticotropin; adrenocorticotropic hormone</td>
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<tr>
<td>Ade</td>
<td>adenine</td>
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<tr>
<td>Ado</td>
<td>adenosine</td>
</tr>
<tr>
<td>ADP</td>
<td>adenosine 5'-diphosphate</td>
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<tr>
<td>AES</td>
<td>atomic emission spectroscopy</td>
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<tr>
<td>AES</td>
<td>Auger electron spectroscopy</td>
</tr>
<tr>
<td>af</td>
<td>audio frequency</td>
</tr>
<tr>
<td>AFM</td>
<td>atomic force microscopy</td>
</tr>
<tr>
<td>AFS</td>
<td>atomic fluorescence spectroscopy</td>
</tr>
<tr>
<td>AGU</td>
<td>anhydroglucose unit</td>
</tr>
<tr>
<td>ala</td>
<td>alanyl in genetics</td>
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<tr>
<td>Ala</td>
<td>alanyl, alanine</td>
</tr>
<tr>
<td>alt</td>
<td>alternating, as in poly(A-alt-B)</td>
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<tr>
<td>AM</td>
<td>amplitude modulation</td>
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<tr>
<td>AMP</td>
<td>adenosine 5'-monophosphate, adenosine 5'-phosphate</td>
</tr>
<tr>
<td>amu</td>
<td>atomic mass unit [amu, reference to oxygen, is deprecated; u (reference to mass of $^{12}$C) should be used]</td>
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<tr>
<td>anal.</td>
<td>analysis (Anal. in combustion analysis presentations)</td>
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<td>anhyd</td>
<td>anhydrous</td>
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<tr>
<td>ANN</td>
<td>artificial neural network</td>
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<td>ANOVA</td>
<td>analysis of variance</td>
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<td>Ans</td>
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<td>ansyl</td>
<td>8-anilino-1-naphthalenesulfonyle</td>
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<td>antilog</td>
<td>antilogarithm</td>
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<td>AO</td>
<td>atomic orbital</td>
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<tr>
<td>ap</td>
<td>antiperiplanar</td>
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<tr>
<td>AP</td>
<td>appearance potential</td>
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<tr>
<td>APIMS</td>
<td>atmospheric pressure ionization mass spectrometry</td>
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<tr>
<td>APS</td>
<td>appearance potential spectroscopy</td>
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<tr>
<td>aq</td>
<td>aqueous</td>
</tr>
<tr>
<td>$A_r$</td>
<td>relative atomic mass (atomic weight)</td>
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<td>ary1</td>
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<tr>
<td>AR</td>
<td>analytical reagent (e.g., AR grade)</td>
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<td>Ara</td>
<td>arabinose</td>
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<tr>
<td>ara-A</td>
<td>adenosine, with arabinose rather than ribose (arabinoadenosine, also ara-A, araA)</td>
</tr>
<tr>
<td>ara-C</td>
<td>cytidine, with arabinose rather than ribose (arabinocytidine, also ara-C, araC)</td>
</tr>
<tr>
<td>arb unit</td>
<td>arbitrary unit (clinical)</td>
</tr>
<tr>
<td>Abbreviation</td>
<td>Definition</td>
</tr>
<tr>
<td>--------------</td>
<td>------------</td>
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<tr>
<td>Arg</td>
<td>arginyl, arginine</td>
</tr>
<tr>
<td>ARPES</td>
<td>angle-resolved photoelectron spectroscopy</td>
</tr>
<tr>
<td>ARPS</td>
<td>angle-resolved photoelectron spectroscopy</td>
</tr>
<tr>
<td>as</td>
<td>asymmetrical</td>
</tr>
<tr>
<td>AS</td>
<td>absorption spectroscopy</td>
</tr>
<tr>
<td>Asa</td>
<td>β-carboxyaspartic acid</td>
</tr>
<tr>
<td>ASIS</td>
<td>aromatic solvent-induced shift</td>
</tr>
<tr>
<td>Asn</td>
<td>asparaginyl, asparagine</td>
</tr>
<tr>
<td>Asp</td>
<td>aspartyl, aspartic acid</td>
</tr>
<tr>
<td>Asx</td>
<td>“Asn or Asp”</td>
</tr>
<tr>
<td>asym</td>
<td>asymmetrical</td>
</tr>
<tr>
<td>at. wt</td>
<td>atomic weight</td>
</tr>
<tr>
<td>ATCC</td>
<td>American Type Culture Collection</td>
</tr>
<tr>
<td>atm</td>
<td>atmosphere</td>
</tr>
<tr>
<td>atom %</td>
<td>atom percent</td>
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<tr>
<td>ATP</td>
<td>adenosine 5’-triphosphate</td>
</tr>
<tr>
<td>ATPase</td>
<td>adenosinetriphosphatase</td>
</tr>
<tr>
<td>ATR</td>
<td>attenuated total reflection</td>
</tr>
<tr>
<td>au</td>
<td>atomic unit</td>
</tr>
<tr>
<td>AU</td>
<td>absorbance unit</td>
</tr>
<tr>
<td>AUFS</td>
<td>absorbance units at full scale</td>
</tr>
<tr>
<td>av</td>
<td>average</td>
</tr>
<tr>
<td>β</td>
<td>stereochemical descriptor</td>
</tr>
<tr>
<td>b</td>
<td>barn (neutron capture area, 10⁻²⁴ cm²)</td>
</tr>
<tr>
<td></td>
<td>bohr (unit of length)</td>
</tr>
<tr>
<td></td>
<td>broad or broadened (spectra)</td>
</tr>
<tr>
<td>b</td>
<td>b axis</td>
</tr>
<tr>
<td></td>
<td>block, as in poly(A-b-B)</td>
</tr>
<tr>
<td>B</td>
<td>“aspartic acid or asparagine”</td>
</tr>
<tr>
<td>bel</td>
<td>buckingham (10⁻²⁶ esu cm²)</td>
</tr>
<tr>
<td></td>
<td>ring (italic in steroid names)</td>
</tr>
<tr>
<td>B</td>
<td>boat (conformation)</td>
</tr>
<tr>
<td>B.C.</td>
<td>before Christ</td>
</tr>
<tr>
<td>B.C.E.</td>
<td>before the common era</td>
</tr>
<tr>
<td>b.i.d.</td>
<td>twice a day</td>
</tr>
<tr>
<td>bar</td>
<td>unit of pressure; unit and abbreviation are the same</td>
</tr>
<tr>
<td>bbl</td>
<td>barrel</td>
</tr>
<tr>
<td>bcc</td>
<td>body-centered cubic (crystal structure)</td>
</tr>
<tr>
<td>bccub</td>
<td>body-centered cubic (crystal structure)</td>
</tr>
<tr>
<td>BCD</td>
<td>binary coded decimal</td>
</tr>
<tr>
<td>Bd</td>
<td>baud</td>
</tr>
<tr>
<td>BEHP</td>
<td>bis(2-ethylhexyl) phthalate</td>
</tr>
<tr>
<td>BET</td>
<td>Brunauer–Emmett–Teller (adsorption isotherm)</td>
</tr>
<tr>
<td>BeV</td>
<td>billion electronvolts</td>
</tr>
<tr>
<td>Abbreviation</td>
<td>Description</td>
</tr>
<tr>
<td>--------------</td>
<td>-------------</td>
</tr>
<tr>
<td>bGH</td>
<td>bovine growth hormone</td>
</tr>
<tr>
<td>Bi</td>
<td>biot</td>
</tr>
<tr>
<td>binap</td>
<td>2,2'-bis(diphenylphosphino)-1,1'-binaphthyl (ligand)</td>
</tr>
<tr>
<td>binol</td>
<td>1,1'-bi-2-naphthol (ligand)</td>
</tr>
<tr>
<td>biol</td>
<td>biological(ly)</td>
</tr>
<tr>
<td>bipy</td>
<td>2,2'-bipyridine, 2,2''-bipyridyl (bpy preferred)</td>
</tr>
<tr>
<td></td>
<td>4,4'-bipyridine, 4,4''-bipyridyl (bpy preferred)</td>
</tr>
<tr>
<td>bis-Tris</td>
<td>[bis(2-hydroxyethyl)amino]tris(hydroxymethyl)methane (also bistris, Bis-Tris, bis-tris)</td>
</tr>
<tr>
<td>bit</td>
<td>binary digit</td>
</tr>
<tr>
<td>BL</td>
<td>bioluminescence</td>
</tr>
<tr>
<td>BM</td>
<td>Bohr magneton (use $\mu_B$)</td>
</tr>
<tr>
<td>Bn</td>
<td>benzyl (also Bzl)</td>
</tr>
<tr>
<td>BN</td>
<td>bond number</td>
</tr>
<tr>
<td>BO</td>
<td>Born–Oppenheimer</td>
</tr>
<tr>
<td>BOD</td>
<td>biological oxygen demand</td>
</tr>
<tr>
<td>bp</td>
<td>base pair</td>
</tr>
<tr>
<td></td>
<td>boiling point</td>
</tr>
<tr>
<td>bps</td>
<td>bits per second</td>
</tr>
<tr>
<td>Bps</td>
<td>bytes per second</td>
</tr>
<tr>
<td>bpy</td>
<td>2,2'-bipyridine, 2,2''-bipyridyl</td>
</tr>
<tr>
<td></td>
<td>4,4'-bipyridine, 4,4''-bipyridyl</td>
</tr>
<tr>
<td>BPY</td>
<td>bipyramidal (coordination compounds)</td>
</tr>
<tr>
<td>Bq</td>
<td>becquerel</td>
</tr>
<tr>
<td>br</td>
<td>broad or broadened (spectra)</td>
</tr>
<tr>
<td>BSA</td>
<td>bovine serum albumin</td>
</tr>
<tr>
<td>BSSE</td>
<td>basis set superposition error</td>
</tr>
<tr>
<td>Btu</td>
<td>British thermal unit</td>
</tr>
<tr>
<td>bu</td>
<td>bushel</td>
</tr>
<tr>
<td>Bu</td>
<td>butyl</td>
</tr>
<tr>
<td>BWR</td>
<td>Benedict–Webb–Rubin (equation)</td>
</tr>
<tr>
<td>Bz</td>
<td>benzoyl</td>
</tr>
<tr>
<td>Bzac</td>
<td>benzoyleacetone</td>
</tr>
<tr>
<td>Bzl</td>
<td>benzyl (also Bn)</td>
</tr>
<tr>
<td>$\chi$</td>
<td>magnetic susceptibility</td>
</tr>
<tr>
<td>c</td>
<td>candle</td>
</tr>
<tr>
<td></td>
<td>centered (crystal structure)</td>
</tr>
<tr>
<td></td>
<td>centi ($10^{-2}$)</td>
</tr>
<tr>
<td></td>
<td>cyclo [as in c-C$<em>6$H$</em>{11}$, c-Hx (cyclohexyl)]</td>
</tr>
<tr>
<td>$c$</td>
<td>c axis</td>
</tr>
<tr>
<td></td>
<td>concentration, for rotation, e.g., $[\alpha]_{489}^2$ +25 (c 0.13, CHCl$_3$)</td>
</tr>
<tr>
<td></td>
<td>cyclo [as in c-S$_6$ (cyclo-hexasulfur)]</td>
</tr>
<tr>
<td></td>
<td>specific cytochrome (i.e., cytochrome c)</td>
</tr>
<tr>
<td>C</td>
<td>Celsius (use $^\circ$C as unit abbreviation)</td>
</tr>
<tr>
<td></td>
<td>coulomb</td>
</tr>
<tr>
<td></td>
<td>cysteine</td>
</tr>
<tr>
<td>Term</td>
<td>Definition</td>
</tr>
<tr>
<td>------</td>
<td>------------</td>
</tr>
<tr>
<td>C</td>
<td>cytidine ring (italic in steroid names)</td>
</tr>
<tr>
<td>C</td>
<td>chair (conformation)</td>
</tr>
<tr>
<td>C.E.</td>
<td>common era</td>
</tr>
<tr>
<td>c/m²</td>
<td>candles per square meter</td>
</tr>
<tr>
<td>¹³C NMR</td>
<td>carbon nuclear magnetic resonance</td>
</tr>
<tr>
<td>ca.</td>
<td>circa, about [used before an approximate date or figure (ca. 1960)]</td>
</tr>
<tr>
<td>CAD</td>
<td>computer-assisted design</td>
</tr>
<tr>
<td>cal</td>
<td>calorie</td>
</tr>
<tr>
<td>cal₄T</td>
<td>International Table calorie</td>
</tr>
<tr>
<td>calcd</td>
<td>calculated</td>
</tr>
<tr>
<td>CAM</td>
<td>computer-assisted manufacturing</td>
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<tr>
<td>cAMP</td>
<td>adenosine cyclic 3′,5′-phosphate</td>
</tr>
<tr>
<td>CAN</td>
<td>ceric ammonium nitrate</td>
</tr>
<tr>
<td>CARS</td>
<td>coherent anti-Stokes Raman spectroscopy</td>
</tr>
<tr>
<td>CAT</td>
<td>computed axial tomography</td>
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<tr>
<td>cB</td>
<td>conjugate base, counterbase (also CB)</td>
</tr>
<tr>
<td>Cbz</td>
<td>carbobenzoxy, carbobenzyloxy, (benzyloxy)carbonyl, benzyl-oxycarbonyl (also Z)</td>
</tr>
<tr>
<td>cc</td>
<td>cubic centimeter (do not use; use cm³ or mL)</td>
</tr>
<tr>
<td>CCD</td>
<td>charge-coupled device</td>
</tr>
<tr>
<td>CCGC</td>
<td>capillary column gas chromatography</td>
</tr>
<tr>
<td>ccp</td>
<td>cubic close-packed (crystal structure)</td>
</tr>
<tr>
<td>cd</td>
<td>candela</td>
</tr>
<tr>
<td>CD</td>
<td>circular dichroism</td>
</tr>
<tr>
<td>CDH</td>
<td>ceramide dihexoside [Cer(Hex)₂]</td>
</tr>
<tr>
<td>cDNA</td>
<td>complementary DNA</td>
</tr>
<tr>
<td>CDP</td>
<td>cytidine 5′-diphosphate</td>
</tr>
<tr>
<td>CE</td>
<td>Cotton effect</td>
</tr>
<tr>
<td>CE–MS</td>
<td>capillary electrophoresis–mass spectrometry</td>
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<tr>
<td>cf.</td>
<td>compare</td>
</tr>
<tr>
<td>CFC</td>
<td>chlorofluorocarbon</td>
</tr>
<tr>
<td>cfm</td>
<td>cubic feet per minute</td>
</tr>
<tr>
<td>CFSE</td>
<td>crystal field stabilization energy (also cfse)</td>
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<tr>
<td>cfu</td>
<td>colony-forming units (bacterial inocula)</td>
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<tr>
<td>cgs</td>
<td>centimeter–gram–second (as in cgs system)</td>
</tr>
<tr>
<td>cgsu</td>
<td>centimeter–gram–second unit(s)</td>
</tr>
<tr>
<td>ChE</td>
<td>cholinesterase</td>
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<tr>
<td>CHF</td>
<td>coupled Hartree–Fock</td>
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<tr>
<td>Ci</td>
<td>curie</td>
</tr>
<tr>
<td>CI</td>
<td>chemical ionization</td>
</tr>
<tr>
<td>CIDE</td>
<td>configuration interaction</td>
</tr>
<tr>
<td>CIDE</td>
<td>chemically induced dynamic electron polarization</td>
</tr>
<tr>
<td>Term</td>
<td>Definition</td>
</tr>
<tr>
<td>------</td>
<td>------------</td>
</tr>
<tr>
<td>CIDNP</td>
<td>chemically induced dynamic nuclear polarization</td>
</tr>
<tr>
<td>CIMS</td>
<td>chemical ionization mass spectrometry</td>
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<tr>
<td>CL</td>
<td>cathodoluminescence</td>
</tr>
<tr>
<td></td>
<td>chemiluminescence</td>
</tr>
<tr>
<td>CM</td>
<td>carboxymethyl (as in CM-cellulose)</td>
</tr>
<tr>
<td>cmc</td>
<td>critical micelle concentration</td>
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<tr>
<td>CMH</td>
<td>ceramide monohexoside [Cer(Hex)]</td>
</tr>
<tr>
<td>CMO</td>
<td>canonical molecular orbital</td>
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<tr>
<td>CMP</td>
<td>cytidine 5’-monophosphate, cytidine 5’-phosphate</td>
</tr>
<tr>
<td>cmr</td>
<td>carbon magnetic resonance <em>(do not use; use $^{13}$C NMR)</em></td>
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<tr>
<td>CMR</td>
<td>carbon magnetic resonance <em>(do not use; use $^{13}$C NMR)</em></td>
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<tr>
<td>CN</td>
<td>coordination number</td>
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<tr>
<td>CNDO</td>
<td>complete neglect of differential overlap</td>
</tr>
<tr>
<td>CNS</td>
<td>central nervous system</td>
</tr>
<tr>
<td>co</td>
<td>copoly (as in A-co-B)</td>
</tr>
<tr>
<td>CoA</td>
<td>coenzyme A</td>
</tr>
<tr>
<td>cod</td>
<td>1,5-cyclooctadiene (ligand)</td>
</tr>
<tr>
<td>COD</td>
<td>chemical oxygen demand</td>
</tr>
<tr>
<td>coeff</td>
<td>coefficient</td>
</tr>
<tr>
<td>colog</td>
<td>cologarithm</td>
</tr>
<tr>
<td>compd</td>
<td>compound</td>
</tr>
<tr>
<td>con</td>
<td>conrotatory (may be italic)</td>
</tr>
<tr>
<td>concd</td>
<td>concentrated</td>
</tr>
<tr>
<td>concn</td>
<td>concentration</td>
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<td>corrected</td>
</tr>
<tr>
<td>cos</td>
<td>cosine</td>
</tr>
<tr>
<td>cosh</td>
<td>hyperbolic cosine</td>
</tr>
<tr>
<td>COSY</td>
<td>correlation spectroscopy</td>
</tr>
<tr>
<td>cot</td>
<td>cotangent</td>
</tr>
<tr>
<td></td>
<td>1,3,5,7-cyclooctatetraene (ligand)</td>
</tr>
<tr>
<td>coth</td>
<td>hyperbolic cotangent</td>
</tr>
<tr>
<td>counts/s</td>
<td>counts per second</td>
</tr>
<tr>
<td>$C_p$</td>
<td>heat capacity at constant pressure</td>
</tr>
<tr>
<td>cp</td>
<td>candlepower</td>
</tr>
<tr>
<td>cP</td>
<td>centipoise</td>
</tr>
<tr>
<td>Cp</td>
<td>cyclopentadienyl</td>
</tr>
<tr>
<td>CP</td>
<td>chemically pure</td>
</tr>
<tr>
<td>CP/MAS</td>
<td>cross-polarization/magic-angle spinning (also CP-MAS, CP–MAS, CPMAS, CP MAS)</td>
</tr>
<tr>
<td>cpd</td>
<td>contact potential difference</td>
</tr>
<tr>
<td>CPE</td>
<td>controlled-potential electrolysis</td>
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<tr>
<td>CPK</td>
<td>Corey–Pauling–Koltun (molecular models)</td>
</tr>
<tr>
<td></td>
<td>creatine phosphokinase</td>
</tr>
<tr>
<td>CPL</td>
<td>circular polarization of luminescence</td>
</tr>
<tr>
<td>cpm</td>
<td>counts per minute</td>
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</table>
cps  counts per second (use counts/s)
cycles per second (use Hz or s⁻¹)
CRAMPS  combined rotation and multiple-pulse spectroscopy
CRIMS  chemical reaction interface mass spectrometry
crit  critical
cRNA  complementary RNA
CRT  cathode ray tube
CRU  constitutional repeating unit
cyst  crystalline
csc  cosecant
csch  hyperbolic cosecant
CT  charge transfer
CTEM  conventional transmission electron microscopy
CTH  ceramide trihexoside [Cer(Hex)₃]
CTP  cytidine 5’-triphosphate
CU-8  cubic, coordination number 8
Cub  cubic (crystal structure)
Cᵥ  heat capacity at constant volume
CV  coefficient of variation
cyclic voltammetry
CVD  chemical vapor deposition
CW  constant width
continuous wave (as in CW ESR)
cwt  hundredweight
Cy  cyclohexyl
cyclam  1,4,8,11-tetraazacyclotetradecane
Cyd  cytidine
Cys  cysteinyl, cysteine
cyt  cytochrome
Cyt  cytosine
cyRNA  cytoplasmic RNA
CZE  capillary zone electrophoresis

δ  NMR chemical shift in parts per million downfield from a standard
∂  partial differential
d  day (spelled-out form is preferred)
  deci (10⁻¹)
  deoxy
  deuteron
differential (mathematical)
diffuse
doublet (spectra)
d.  diameter, with i. and o. (inside and outside)
density
d  distance
  dextrorotatory
  spacing (X-ray)
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>d</td>
<td>absolute configuration</td>
</tr>
<tr>
<td>D</td>
<td>aspartic acid</td>
</tr>
<tr>
<td></td>
<td>debye</td>
</tr>
<tr>
<td></td>
<td>deuterium</td>
</tr>
<tr>
<td>ring (italic in steroid names)</td>
<td></td>
</tr>
<tr>
<td>D</td>
<td>diffusion coefficient</td>
</tr>
<tr>
<td></td>
<td>symmetry group [e.g., $D_3$; also used in names, such as (+)-$D_3$-tris-homocubane]</td>
</tr>
<tr>
<td>2-D</td>
<td>two-dimensional (also 2D)</td>
</tr>
<tr>
<td>3-D</td>
<td>three-dimensional (also 3D)</td>
</tr>
<tr>
<td>da</td>
<td>deca or deka (10)</td>
</tr>
<tr>
<td>Da</td>
<td>dalton</td>
</tr>
<tr>
<td>daf</td>
<td>dry ash free</td>
</tr>
<tr>
<td>dAMP</td>
<td>2′-deoxyadenosine 5′-monophosphate or phosphate (the A can be replaced with C, G, U, etc.)</td>
</tr>
<tr>
<td>dansyl</td>
<td>5-(dimethylamino)-1-naphthalenesulfonyl</td>
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<tr>
<td>dB</td>
<td>decibel</td>
</tr>
<tr>
<td>dc</td>
<td>direct current</td>
</tr>
<tr>
<td>DD-8</td>
<td>dodecahedral, coordination number 8</td>
</tr>
<tr>
<td>DD NMR</td>
<td>dipolar decoupling NMR</td>
</tr>
<tr>
<td>DDT</td>
<td>1,1,1-trichloro-2,2-bis($p$-chlorophenyl)ethane</td>
</tr>
<tr>
<td>de</td>
<td>diastereomeric excess</td>
</tr>
<tr>
<td>DEAE</td>
<td>(diethylamino)ethyl (as in DEAE-cellulose)</td>
</tr>
<tr>
<td>dec</td>
<td>decomposition</td>
</tr>
<tr>
<td>decomp</td>
<td>decompose</td>
</tr>
<tr>
<td>DEFT</td>
<td>driven equilibrium Fourier transform</td>
</tr>
<tr>
<td>deg</td>
<td>degree (use °B, degrees Baumé; °C, °F, but K)</td>
</tr>
<tr>
<td>DEG</td>
<td>diethylene glycol</td>
</tr>
<tr>
<td>DEHP</td>
<td>bis(2-ethylhexyl) phthalate (BEHP is preferred)</td>
</tr>
<tr>
<td>DES</td>
<td>diethylstilbestrol</td>
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<tr>
<td>det</td>
<td>determinant</td>
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<tr>
<td>df</td>
<td>degrees of freedom</td>
</tr>
<tr>
<td>DF</td>
<td>degrees of freedom</td>
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<tr>
<td>DFT</td>
<td>density functional theory</td>
</tr>
<tr>
<td>diam</td>
<td>diameter</td>
</tr>
<tr>
<td>dil</td>
<td>dilute</td>
</tr>
<tr>
<td>dis</td>
<td>disrotatory (may be italic)</td>
</tr>
<tr>
<td>distd</td>
<td>distilled</td>
</tr>
<tr>
<td>DLVO</td>
<td>Derjaguin–Landau–Verwey–Overbeek</td>
</tr>
<tr>
<td>DMA</td>
<td>dynamic mechanical analyzer</td>
</tr>
<tr>
<td>DMBA</td>
<td>9,10-dimethylbenz[a]anthracene</td>
</tr>
<tr>
<td>DME</td>
<td>1,2-dimethoxyethane</td>
</tr>
<tr>
<td></td>
<td>dropping mercury electrode</td>
</tr>
<tr>
<td>DMEM</td>
<td>Dulbecco's modified Eagle's medium</td>
</tr>
<tr>
<td>DMF</td>
<td>dimethylformamide</td>
</tr>
<tr>
<td>DMN</td>
<td>diaminomaleonitrile</td>
</tr>
<tr>
<td>dmr</td>
<td>deuterium magnetic resonance (do not use; use $^2$H NMR)</td>
</tr>
<tr>
<td>Abbreviation</td>
<td>Full Form</td>
</tr>
<tr>
<td>--------------</td>
<td>-----------</td>
</tr>
<tr>
<td>DMR</td>
<td>deuterium magnetic resonance (do not use; use $^2$H NMR)</td>
</tr>
<tr>
<td>DMSO</td>
<td>dimethyl sulfoxide (also Me$_2$SO)</td>
</tr>
<tr>
<td>DMTA</td>
<td>dynamic mechanical thermal analyzer</td>
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<tr>
<td>DNA</td>
<td>deoxyribonucleic acid</td>
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<tr>
<td>DNase</td>
<td>deoxyribonuclease</td>
</tr>
<tr>
<td>DNMR</td>
<td>dynamic nuclear magnetic resonance</td>
</tr>
<tr>
<td>DNP</td>
<td>deoxynucleoprotein</td>
</tr>
<tr>
<td>DNPH</td>
<td>(2,4-dinitrophenyl)hydrazine</td>
</tr>
<tr>
<td>Dns</td>
<td>dansyl</td>
</tr>
<tr>
<td>Dopa</td>
<td>3-(3,4-dihydroxyphenyl)alanine (also DOPA)</td>
</tr>
<tr>
<td>DP</td>
<td>degree of polymerization (also dp)</td>
</tr>
<tr>
<td>dpm</td>
<td>disintegrations per minute</td>
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<tr>
<td>DPPH</td>
<td>2,2-diphenyl-1-picrylhydrazyl</td>
</tr>
<tr>
<td>dps</td>
<td>disintegrations per second</td>
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<tr>
<td>D$q$</td>
<td>crystal field splittings</td>
</tr>
<tr>
<td>DQF</td>
<td>double quantum filtered</td>
</tr>
<tr>
<td>DRIFT</td>
<td>diffuse reflectance Fourier transform</td>
</tr>
<tr>
<td>D$s$</td>
<td>crystal field splittings</td>
</tr>
<tr>
<td>DSC</td>
<td>differential scanning calorimetry</td>
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<tr>
<td>dT</td>
<td>thymidine</td>
</tr>
<tr>
<td>D$t$</td>
<td>crystal field splittings</td>
</tr>
<tr>
<td>DTA</td>
<td>differential thermal analysis</td>
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<tr>
<td>DTC</td>
<td>depolarization thermocurrent</td>
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<td>dTDP</td>
<td>thymidine 5’-diphosphate</td>
</tr>
<tr>
<td>DTE</td>
<td>dithioerythritol</td>
</tr>
<tr>
<td>dThd</td>
<td>thymidine</td>
</tr>
<tr>
<td>dTMP</td>
<td>thymidine 5’-monophosphate, thymidine 5’-phosphate</td>
</tr>
<tr>
<td>DTT</td>
<td>dithiothreitol</td>
</tr>
<tr>
<td>dTTP</td>
<td>thymidine 5’-triphosphate</td>
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<tr>
<td>dyn</td>
<td>dyne</td>
</tr>
<tr>
<td>$\varepsilon$</td>
<td>dielectric constant</td>
</tr>
<tr>
<td>$\varepsilon^*$</td>
<td>complex permittivity</td>
</tr>
<tr>
<td>$e$</td>
<td>base of natural logarithm</td>
</tr>
<tr>
<td>$e^{-}$</td>
<td>electron</td>
</tr>
<tr>
<td>$e_{aq}^{-}$</td>
<td>hydrated electron</td>
</tr>
<tr>
<td>$e^{-}(aq)$</td>
<td>hydrated electron</td>
</tr>
<tr>
<td>$e_{s}^{-}$</td>
<td>solvated electron</td>
</tr>
<tr>
<td>$e^{-}(s)$</td>
<td>solvated electron</td>
</tr>
<tr>
<td>$e$</td>
<td>electronic charge</td>
</tr>
<tr>
<td>E</td>
<td>exa (10$^{18}$) glutamic acid</td>
</tr>
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</table>
$E$  electromotive force
   energy
   entgegen (configuration)
   envelope (conformation)
   potential energy
   specific extinction coefficient ($E_{280}^{1\%{c},1cm}$)
   Young’s modulus
$E^o$  standard electrode potential
   standard electromotive force
$E_{1/2}$  half-wave potential
$E_1$  first-order elimination
$E_2$  second-order elimination
   e.g.  for example
$E_a, E_A$  Arrhenius or activation energy
$ea_0$  electronic charge in electrostatic units $\times$ Bohr radius or atomic units
   for dipole moment
EC  exclusion chromatography
EDC  electron-capture detector, detection
ECE  electrochemical, chemical, electrochemical (mechanisms)
ECG  electrocardiogram
ecl  electrochemical luminescence
ECL  electrochemical luminescence
ECP  effective core potential
ed.  edition, edited
Ed.  editor
ED  effective dose
ED_{50}  dose that is effective in 50% of test subjects (also ED50)
edda  ethylenediaminediaceto (ligand)
eds.  editions
Eds.  editors
EDS  energy-dispersive system (or spectrometry)
edta  ethylenediaminetetraacetato (ligand)
EDTA  ethylenediaminetetraacetic acid, ethylenediaminetetraacetate
EDXS  energy-dispersive X-ray spectrometry
ee  enantiomeric excess
EEG  electroencephalogram
EELS  electron energy loss spectroscopy
EFG  electric field gradient
EGA  evolved gas analysis
EGD  evolved gas detection
EGR  exhaust gas recirculation
$E_h$  hartree (unit); Hartree energy
EH  extended Hückel
EI  electron impact
   electron ionization
EIA  enzyme immunoassay
$E_k$  kinetic energy
EKC  electrokinetic chromatography
EKG  electrocardiogram
EL  electroluminescence
ELISA  enzyme-linked immunosorbent (immunoadsorbent) assay
e/m  ratio of electron charge to mass
EM  electron microscopy
e-mail  electronic mail
EMC  equilibrium moisture content
emf  electromotive force
EMIS  electromagnetic isotope separation
emu  electromagnetic unit
en  ethylenediamine (ligand)
ENDOR  electron–nuclear double resonance
ent  reversal of stereocenters
Ep  potential energy
EPA  ether–isopentane–ethanol (solvent system)
epi  inversion of normal configuration (italic with a number, as in 15-epi-
       prostaglandin A)
EPMA  electron probe microanalysis
EPR  electron paramagnetic resonance
EPXMA  electron probe X-ray microanalysis
eq  equation
equiv  equivalent
equiv wt  equivalent weight
erf  error function
erfc  error function complement
erfc⁻¹  inverse error function complement
ESCA  electron spectroscopy for chemical analysis
esd  estimated standard deviation
ESE  electron spin echo
ESEEM  electron spin echo envelope modulation
ESI  electrospray ionization
ESIMS  electrospray ionization mass spectrometry
ESP  elimination of solvation procedure
ESR  electron spin resonance
esu  electrostatic unit
Et  ethyl
et al.  and others
etc.  and so forth
eu  entropy unit
EU  enzyme unit
eV  electronvolt
EXAFS  extended X-ray absorption fine structure
exch  exchangeable (spectra)
exp  exponential
expt  experiment
exptl  experimental
f and page following (as in p 457 f)

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tr>
<td>femto</td>
<td>$10^{-15}$</td>
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<tr>
<td>fermi</td>
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<tr>
<td>fine</td>
<td>spectral</td>
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$f$

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<tr>
<td>focal length</td>
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</tr>
<tr>
<td>frequency (in statistics)</td>
<td></td>
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<tr>
<td>function [as in $f(x)$]</td>
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<tr>
<td>furanose form</td>
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$F$

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<tr>
<td>Fahrenheit</td>
<td>$°$F as unit abbreviation</td>
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<tr>
<td>farad</td>
<td></td>
</tr>
<tr>
<td>formal</td>
<td>judiciously; M is preferred</td>
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<tr>
<td>phenylalanine</td>
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$F$

<table>
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<tbody>
<tr>
<td>Faraday constant</td>
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<tr>
<td>variance ratio (in statistics)</td>
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<table>
<thead>
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<tr>
<td>FAAS</td>
<td>flame atomic absorption spectroscopy</td>
</tr>
<tr>
<td>FABMS</td>
<td>fast atom bombardment mass spectrometry</td>
</tr>
<tr>
<td>fac</td>
<td>facial</td>
</tr>
<tr>
<td>FAD</td>
<td>flavin adenine dinucleotide</td>
</tr>
<tr>
<td>FAES</td>
<td>flame atomic emission spectroscopy</td>
</tr>
<tr>
<td>FAFS</td>
<td>flame atomic fluorescence spectroscopy</td>
</tr>
<tr>
<td>FAS</td>
<td>flame absorption spectroscopy</td>
</tr>
<tr>
<td>fcc</td>
<td>face-centered cubic (crystal structure)</td>
</tr>
<tr>
<td>FCC</td>
<td>fluid catalytic cracking</td>
</tr>
<tr>
<td>Fd</td>
<td>ferredoxin</td>
</tr>
<tr>
<td>FEM</td>
<td>field emission microscopy or spectroscopy</td>
</tr>
<tr>
<td>FES</td>
<td>field emission spectroscopy</td>
</tr>
<tr>
<td>FID</td>
<td>flame emission spectrometry</td>
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<table>
<thead>
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<th>Description</th>
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<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<td>FFEM</td>
<td>freeze–fracture electron microscopy</td>
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<tr>
<td>FFF</td>
<td>field flow fractionation</td>
</tr>
<tr>
<td>FFS</td>
<td>flame fluorescence spectroscopy</td>
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<tr>
<td>FFT</td>
<td>fast Fourier transform</td>
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<tr>
<td>FHT</td>
<td>Fisher–Hirschfelder–Taylor (space-filling models)</td>
</tr>
<tr>
<td>FI</td>
<td>field ionization</td>
</tr>
<tr>
<td>FIA</td>
<td>flow-injection analysis</td>
</tr>
<tr>
<td>fid</td>
<td>free induction decay (in Fourier transform work)</td>
</tr>
<tr>
<td>FID</td>
<td>flame ionization detector, detection</td>
</tr>
<tr>
<td>FIK</td>
<td>field ionization kinetics</td>
</tr>
<tr>
<td>FIR</td>
<td>far-infrared</td>
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<tr>
<td>FLC</td>
<td>ferroelectric liquid crystal</td>
</tr>
<tr>
<td>fm</td>
<td>femtometer</td>
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<tr>
<td>fm</td>
<td>fermi (unit of length, also f)</td>
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</table>

<table>
<thead>
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<th>Symbol</th>
<th>Description</th>
</tr>
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<tbody>
<tr>
<td>FM</td>
<td>frequency modulation</td>
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<tr>
<td>FMN</td>
<td>flavin mononucleotide</td>
</tr>
<tr>
<td>FMO</td>
<td>frontier molecular orbital</td>
</tr>
</tbody>
</table>
Chapter 10: Editorial Style

FOPPA  first-order polarization propagator approach
fp     freezing point
FPC    fixed partial charge
FPT    finite perturbation theory
Fr     franklin
Fr     Froude number
Fru    fructose
FSGO   floating spherical Gaussian orbital
FSH    follicle-stimulating hormone
ft     foot
FT     Fourier transform
ft-c   foot-candle
ft-lb  foot-pound
ft-lbf  foot-pound-force
FTICR  Fourier transform ion cyclotron resonance
FTIR   Fourier transform infrared (also FT/IR, FT-IR, and FT IR)
FTIRS  Fourier transform infrared spectroscopy
FTP    file transfer protocol
FTS    Fourier transform spectroscopy
Fuc    fucose
fw     formula weight
fwhh   full width at half-height
fwhm   full width at half-maximum

γ  microgram (use µg)
    photon
    surface tension
Γ  surface concentration
g  gas [as in H₂O(g)]
    gram
    acceleration due to gravity (closed up to number preceding)
    splitting factor (ESR and NMR spectroscopy)
G  gauss
    generally labeled
    giga (10⁹)
    glycine
    guanosine
G  Gibbs energy
    gravitational constant
g-atom  gram-atom (use mol)
Ga     Galileo number
gal    gallon
Gal    galactose
GalNAc N-acetylgalactosamine
GC     gas chromatography
GDC    gas displacement chromatography
<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
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<tbody>
<tr>
<td>GDMS</td>
<td>glow discharge mass spectrometry</td>
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<tr>
<td>GDP</td>
<td>guanosine 5’-diphosphate</td>
</tr>
<tr>
<td>gem</td>
<td>geminal</td>
</tr>
<tr>
<td>GFAAS</td>
<td>graphite furnace atomic absorption spectroscopy</td>
</tr>
<tr>
<td>GFC</td>
<td>gas frontal chromatography</td>
</tr>
<tr>
<td>gfw</td>
<td>gram formula weight</td>
</tr>
<tr>
<td>GH</td>
<td>growth hormone (somatotropin)</td>
</tr>
<tr>
<td>GHz</td>
<td>gigahertz</td>
</tr>
<tr>
<td>Gi</td>
<td>gilbert</td>
</tr>
<tr>
<td>GIAO</td>
<td>gauge-invariant atomic orbital</td>
</tr>
<tr>
<td>Glc</td>
<td>glucose</td>
</tr>
<tr>
<td>GLC</td>
<td>gas–liquid chromatography</td>
</tr>
<tr>
<td>GlcNAc</td>
<td>N-acetylglycosamine</td>
</tr>
<tr>
<td>Gln</td>
<td>glutaminyl, glutamine</td>
</tr>
<tr>
<td>GLPC</td>
<td>gas–liquid partition chromatography</td>
</tr>
<tr>
<td>Glu</td>
<td>glutamyl, glutamic acid</td>
</tr>
<tr>
<td>Glx</td>
<td>“Gln or Glu”</td>
</tr>
<tr>
<td>gly</td>
<td>glycine (ligand)</td>
</tr>
<tr>
<td>Gly</td>
<td>glycyll, glycine</td>
</tr>
<tr>
<td>GMP</td>
<td>guanosine 5’-monophosphate, guanosine 5’-phosphate</td>
</tr>
<tr>
<td>GPC</td>
<td>gel permeation chromatography</td>
</tr>
<tr>
<td>gr</td>
<td>grain (unit of weight)</td>
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<tr>
<td>GSC</td>
<td>gas–solid chromatography</td>
</tr>
<tr>
<td>GSH</td>
<td>reduced glutathione</td>
</tr>
<tr>
<td>GSL</td>
<td>glycosphingolipid</td>
</tr>
<tr>
<td>GSSG</td>
<td>oxidized glutathione</td>
</tr>
<tr>
<td>GTP</td>
<td>guanosine 5’-triphosphate</td>
</tr>
<tr>
<td>Gua</td>
<td>guanine</td>
</tr>
<tr>
<td>Guo</td>
<td>guanosine</td>
</tr>
<tr>
<td>Gy</td>
<td>gray (international unit of absorbed dose)</td>
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<table>
<thead>
<tr>
<th>Symbol</th>
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<tr>
<td>η</td>
<td>hapto viscosity</td>
</tr>
<tr>
<td>h</td>
<td>hecto ((10^2)) helion</td>
</tr>
<tr>
<td>h</td>
<td>hour</td>
</tr>
<tr>
<td>h</td>
<td>crystallographic index ((hkl))</td>
</tr>
<tr>
<td>(\hbar)</td>
<td>Planck’s constant</td>
</tr>
<tr>
<td>(\hbar)</td>
<td>Planck’s constant divided by (2\pi)</td>
</tr>
<tr>
<td>H</td>
<td>henry</td>
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<tr>
<td>H</td>
<td>histidine</td>
</tr>
<tr>
<td>(H)</td>
<td>enthalpy</td>
</tr>
<tr>
<td>(\mathcal{H})</td>
<td>half-chair (conformation)</td>
</tr>
<tr>
<td>(\mathcal{H})</td>
<td>Hamiltonian</td>
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<tr>
<td>(^1)H NMR</td>
<td>proton nuclear magnetic resonance</td>
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</tbody>
</table>
2H NMR  deuterium nuclear magnetic resonance
$H_0$  magnetic field (ESR and NMR spectroscopy)
ha  hectare
Hb  hemoglobin
Hbg  biguanide
HCG  human chorionic gonadotropin
hcp  hexagonal close-packed (crystal structure)
HCP  hexachlorophene
HCS  hazard communication standard
HDPE  high-density polyethylene
Hedta  ethylenediaminetetraacetate(3−) (ato as ligand in full name)
H$_2$edta  ethylenediaminetetraacetate(2−) (ato as ligand in full name)
H$_3$edta  ethylenediaminetetraacetate(1−) (ato as ligand in full name)
H$_4$edta  ethylenediaminetetraacetic acid
HEEDTA  N-(2-hydroxyethyl)ethylenediaminetriacetate
Hepes  N-(2-hydroxyethyl)piperazine-N′-ethanesulfonic acid (also HEPES, hepes)
Hepps  N-(2-hydroxyethyl)piperazine-N′-propanesulfonic acid (also HEPPS, hepps)
hex  hexagonal (crystal structure)
HF  Hartree–Fock
hfs  hyperfine splitting
hfsc  hyperfine splitting constant
hGH  human growth hormone
HIPS  high-impact polystyrene
His  histidyl, histidine
HIV  human immunodeficiency virus
hkl  crystallographic index
HMDS  hexamethyldisilane
HEEDTA  hexamethyldisiloxane
HMO  Hückel molecular orbital
HMPA  hexamethylphosphoramide
HMPT  hexamethylphosphoric triamide
hnRNA  heterogeneous nuclear RNA
$hv$  indicates light; $h$ is Planck’s constant, and $\nu$ is the photon frequency
HOHAHA  homonuclear Hartmann–Hahn
HOMO  highest occupied molecular orbital
H$_2$ox  oxalic acid
hp  horsepower
HPCE  high-performance capillary electrophoresis
HPLC  high-performance liquid chromatography
HRM  high-pressure liquid chromatography
HREELS  high-resolution electron energy loss spectroscopy
HREM  high-resolution electron microscopy
HRMS  high-resolution mass spectrometry
HSP  heat shock protein
Hyl  hydroxylysyl, hydroxyllysine
Hyp  hydroxyprolyl, hydroxyproline
hypoxanthine
Hz   hertz

\( i \) \((-1)^{1/2}\)
\( i \)  iso (as in \( i \)-Pr; do not use \( i \)-propyl)
I    inosine
isoleucine

\( I \) electric current (also \( i \))
ionic strength
moment of inertia
spin quantum number (ESR and NMR spectroscopy)
i.d.  inside diameter
i.e.  that is
I/O  input–output
ibid. in the same place (in the reference cited; use is discouraged)
ic  intracerebrally
IC   integrated circuit
ion chromatography
ICP  inductively coupled plasma
ICR  ion cyclotron resonance
ics  internal chemical shift
ICSH interstitial-cell-stimulating hormone
ICT  International Critical Tables
\( i_d \) diffusion current
ID   infective dose
ID_{50} dose that is infective in 50% of test subjects (also ID50)
IDAS isotope dilution \( \alpha \) spectrometry
IDMS isotope dilution mass spectrometry
IDP  inosine 5'-diphosphate
IE   ionization energy
IEC  ion-exchange chromatography
IEF  isoelectric focusing
IEP  isoelectric point
IETS inelastic electron-tunneling spectroscopy
IFQ  interfacial fluorescence quenching
IKES ion kinetic energy spectroscopy
Ile  isoleucyl, isoleucine
ILS  increased life span
im   intramuscularly
IMMA ion microprobe mass analysis
IMP  inosine 5'-monophosphate, inosine 5'-phosphate
in.  inch
INDO intermediate neglect of differential overlap
INDOR internal nuclear double resonance
internucleus (nucleus–nucleus) double resonance
INH inhibitor
isonicotinic acid hydrazide
Ino inosine
INO iterative natural orbital
insol insoluble
ip intraperitoneally
IP ionization potential
ips iron pipe size
IR infrared
IRDO intermediate retention of differential overlap
IRMA immunoradiometric assay
IRMMS isotopic ratio mass spectrometry
IRP internal reflection photolysis
IRRAS infrared reflection–absorption spectroscopy
IRS internal reflection spectroscopy
isc intersystem crossing
ISCA ionization spectroscopy for chemical analysis
ISE ion-selective electrode
iso inversion of normal chirality (not as in isopropyl, but in uses such as
\(8\text{-iso-prostaglandin } E_1\); generally italic with a number)
ISS ion-scattering spectroscopy
ITP inosine 5′-triphosphate
isotachophoresis
IU international unit
iv intravenous, intravenously

J joule
\(J\) coupling constant (NMR and ESR spectroscopy)
JT Jahn–Teller

k kilo \((10^3)\)
\(k\) Boltzmann constant (also \(k_B\))
crystallographic index \((hkl)\)
rate constant

K 1000 (as in 60K protein)
Kayser \(use \text{ cm}^{-1}\)
kelvin \(do not use °K\)
kilobase (kB is preferred)
lysine

\(K\) equilibrium constant
\(K\alpha\) spectral line
kat katal (unit of enzyme catalytic activity)
\(K\beta\) spectral line
\(k_B\) Boltzmann constant
kB kilobase
kilobit
kB  kilobel
    kilobyte
kbar  kilobar
kbp  kilobase pair
kD  kilodebye
kDa  kilodalton
KE  kinetic energy
kg  kilogram
kgf  kilogram-force
kHz  kilohertz

$K_m$  Michaelis constant
$K_{oc}$  carbon-referenced sediment partition coefficient
$K_{oc}$  organic chemicals partition coefficient
$K_{ow}$  octanol–water partition coefficient
$K_{SP}$  solubility product constant
$K_w$  autoionization constant

$\lambda$  absolute activity
    microliter (use $\mu$L)
    wavelength
$\lambda_{ex}$  excitation wavelength
$\lambda_{max}$  wavelength of maximum absorption
l  liquid [as in NH$_3$(l)]
l  crystallographic index (hkl)
levorotatory
L  absolute configuration
L  leucine
    ligand
    liter
$L_1$  spectral line
$L_{II}$  spectral line
$L_{III}$  spectral line
Lac  lactose
LAMMA  laser microprobe mass spectrometry
lat  latitude
lb  pound
lbf  pound-force
LC  liquid chromatography
LCAO  linear combination of atomic orbitals
LCD  liquid-crystal display
LCICD  liquid-crystal-induced circular dichroism
LCVAO  linear combination of virtual atomic orbitals
LD  lethal dose
LD$_{50}$  dose that is lethal to 50% of test subjects (also LD50)
LDH  lactic dehydrogenase
LDMS  laser desorption mass spectrometry
LE  locally excited
LED  light-emitting diode
LEED  low-energy electron diffraction
LEEDS  low-energy electron diffraction spectroscopy
LEISS  low-energy ion-scattering spectroscopy
LEMF  local effective mole fraction
Leu  leucyl, leucine
LFER  linear free-energy relationship
LH  luteinizing hormone
LIF  laser-induced fluorescence
lim  limit
LIMS  laboratory information management system
LIS  lanthanide-induced shift
lit.  literature
LJ, L-J  Lennard-Jones
LLC  liquid–liquid chromatography
lm  lumen
LMCT  ligand-to-metal charge transfer
ln  natural logarithm
LNDO  local neglect of differential overlap
log  logarithm to the base 10
Log  principal logarithm
long.  longitude
Lp  Lorentz–polarization (effect)
Lp  Lorentz factor × polarization factor
LSC  liquid–solid chromatography
LSD  lysergic acid diethylamide
LSR  lanthanide shift reagent
LUMO  lowest unoccupied molecular orbital
lut  lutidine (ligand)
Lut  lutidine
lx  lux
LYP  Lee–Yang–Parr
Lys  lysyl, lysine

µ  chemical potential
dipole moment
electrophoretic mobility
micro (10⁻⁶)
micron (do not use; use µm or micrometer)

µ±  muon
µB  Bohr magneton
µN  nuclear magneton
µW  Weiss magneton
m  medium (spectra)
meter
mile (in mpg and mph; otherwise mi)
milli (10⁻³)
multiplet (spectra)

isotopic mass

magnetic quantum number (ESR and NMR spectroscopy)

m

meta

molal (mol kg⁻¹)

M

mega (10⁶)

mesomeric

metal (do not use Me)

methionine

molar (mol dm⁻³, mol L⁻¹)

M

minus (left-handed helix)

[M]

molecular rotation

m/e

mass-to-charge ratio (m/z is preferred)

mAb

monoclonal antibody (also Mab, MAb)

Mal

maltose

MALDI

matrix-assisted laser desorption ionization

MALDI-TOFMS

matrix-assisted laser desorption ionization time-of-flight mass spectrometry (also MALDI-TOF MS)

Man

mannose

MAO

monoamine oxidase

MAS

magic-angle spinning

MASS

magic-angle sample spinning

max

maximum

Mb

myoglobin

MBE

molecular beam epitaxy

MCD

magnetic circular dichroism

mCi

millicurie

MCT

mercury cadmium telluride

MD

molecular dynamics

melectron rest mass

Me

methyl (not metal)

MED

mean effective dose

MEKC

micellar electrokinetic capillary chromatography

MEM

minimum Eagle’s essential medium

mequiv

milliequivalent

mer

polymer notation (as in 16-mer)

meridional

Mes

mesityl (2,4,6-trimethylphenyl), 2-morpholinoethanesulfonic acid,

2-morpholinoethanesulfonate (also MES)

Met

methionyl, methionine

MetHb

methemoglobin

MetMb

metmyoglobin

MeV

million electronvolts

mho

reciprocal ohm (Ω⁻¹ is preferred)

MHz

megahertz

mi

mile
<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Definition</th>
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<td>min</td>
<td>minimum</td>
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<tr>
<td>minute</td>
<td></td>
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<tr>
<td>MINDO</td>
<td>modified intermediate neglect of differential overlap</td>
</tr>
<tr>
<td>MIR</td>
<td>mid-infrared</td>
</tr>
<tr>
<td>MIRS</td>
<td>multiple internal reflection spectroscopy</td>
</tr>
<tr>
<td>ML</td>
<td>monolayer</td>
</tr>
<tr>
<td>MLCT</td>
<td>metal-to-ligand charge transfer</td>
</tr>
<tr>
<td>MLR</td>
<td>multiple linear regression</td>
</tr>
<tr>
<td>mmHg</td>
<td>millimeters of mercury (measure of pressure)</td>
</tr>
<tr>
<td>mmp</td>
<td>mixture melting point</td>
</tr>
<tr>
<td>mmu</td>
<td>millimass unit</td>
</tr>
<tr>
<td>$m_n$</td>
<td>neutron rest mass</td>
</tr>
<tr>
<td>$M_n$</td>
<td>number-average molecular weight</td>
</tr>
<tr>
<td>MO</td>
<td>molecular orbital</td>
</tr>
<tr>
<td>mol</td>
<td>mole</td>
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<tr>
<td>mol %</td>
<td>mole percent</td>
</tr>
<tr>
<td>molar equiv</td>
<td>molar equivalent</td>
</tr>
<tr>
<td>mol wt</td>
<td>molecular weight ($M_r$ is preferred)</td>
</tr>
<tr>
<td>MOM</td>
<td>methoxymethyl</td>
</tr>
<tr>
<td>mon</td>
<td>monoclinic (crystal structure)</td>
</tr>
<tr>
<td>$m_p$</td>
<td>proton rest mass</td>
</tr>
<tr>
<td>mp</td>
<td>melting point</td>
</tr>
<tr>
<td>MP</td>
<td>Møller–Plesset</td>
</tr>
<tr>
<td>MP2</td>
<td>second-order Møller–Plesset perturbation theory</td>
</tr>
<tr>
<td>mpg</td>
<td>miles per gallon</td>
</tr>
<tr>
<td>mph</td>
<td>miles per hour</td>
</tr>
<tr>
<td>MPI</td>
<td>multiphoton ionization</td>
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<tr>
<td>MPV</td>
<td>Meerwein–Ponndorf–Verley</td>
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<tr>
<td>MQ ENDOR</td>
<td>multiple-quantum electron nuclear double resonance</td>
</tr>
<tr>
<td>$M_r$</td>
<td>relative molecular mass (molecular weight)</td>
</tr>
<tr>
<td>MR</td>
<td>molecular refraction</td>
</tr>
<tr>
<td>MRI</td>
<td>magnetic resonance imaging</td>
</tr>
<tr>
<td>mRNA</td>
<td>messenger RNA</td>
</tr>
<tr>
<td>Ms</td>
<td>mesyl (methylsulfonyl)</td>
</tr>
<tr>
<td>MS</td>
<td>mass spectrometry</td>
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<tr>
<td>mass spectrum</td>
<td></td>
</tr>
<tr>
<td>microwave spectroscopy</td>
<td></td>
</tr>
<tr>
<td>MSDS</td>
<td>manufacturer’s safety data sheet</td>
</tr>
<tr>
<td>material safety data sheet</td>
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</tr>
<tr>
<td>MSG</td>
<td>monosodium glutamate</td>
</tr>
<tr>
<td>MSH</td>
<td>melanocyte-stimulating hormone, melanotropin</td>
</tr>
<tr>
<td>Mt</td>
<td>megaton</td>
</tr>
<tr>
<td>MTD</td>
<td>mean therapeutic dose</td>
</tr>
<tr>
<td>mtDNA</td>
<td>mitochondrial DNA</td>
</tr>
<tr>
<td>mtRNA</td>
<td>mitochondrial RNA</td>
</tr>
<tr>
<td>mu</td>
<td>mass unit</td>
</tr>
</tbody>
</table>
MVA mevalonic acid
MVS multiple-variable storage
$M_w$ weight-average molecular weight
MW molecular weight ($M_r$ is preferred)
MWD molecular weight distribution
Mx maxwell
$M_z$ $z$-average molecular weight
$m/z$ mass-to-charge ratio

ν frequency
$\tilde{\nu}$ wavenumber
$\nu_{1/2}$ full width at half-maximum height (NMR spectra)
$\nu_e$ neutrino
$\nu_{\text{max}}$ frequency of maximum absorption
n nano ($10^{-9}$)
neutron
n normal (as in $n$-butyl, $n$-Bu)
refractive index ($n_{D}^{20}$ at 20 °C, Na D line)
total number of individuals
N asparagine
newton
normal (concentration)
unspecified nucleoside
N.B. nota bene (note well)
$N_A$ Avogadro’s number
NAA neutron activation analysis
[Na]ATPase sodium ion activated ATPase (also Na-ATPase, NaATPase)
NAD nicotinamide adenine dinucleotide
NADH reduced nicotinamide adenine dinucleotide
NADP nicotinamide adenine dinucleotide phosphate
NADPH reduced nicotinamide adenine dinucleotide phosphate
[Na,K]ATPase sodium and potassium ion activated ATPase (also Na,K-ATPase)
NBS $N$-bromosuccinimide
NDA New Drug Application
NDDO neglect of diatomic differential overlap
nDNA nuclear DNA
NEMO nonempirical molecular orbital
neut equiv neutralization equivalent
NHE normal hydrogen electrode
NIR near-infrared
Nle norleucyl, norleucine
NLO nonlinear optical (optics)
nm nanometer
NM nuclear magneton ($use \mu_N$)
NMN nicotinamide mononucleotide
NMR nuclear magnetic resonance (do not use nmr)
no. number
<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Full Form</th>
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<tbody>
<tr>
<td>NO</td>
<td>natural orbital (as in CNDO/2-NO)</td>
</tr>
<tr>
<td>NOCOR</td>
<td>neglect of core orbitals</td>
</tr>
<tr>
<td>NOE</td>
<td>nuclear Overhauser effect</td>
</tr>
<tr>
<td>NOESY</td>
<td>nuclear Overhauser enhancement spectroscopy</td>
</tr>
<tr>
<td>NOx</td>
<td>nitrogen oxides</td>
</tr>
<tr>
<td>Np</td>
<td>neper</td>
</tr>
<tr>
<td>NPR</td>
<td>net protein retention</td>
</tr>
<tr>
<td>NQR</td>
<td>nuclear quadrupole resonance</td>
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<tr>
<td>nRNA</td>
<td>nuclear RNA</td>
</tr>
<tr>
<td>NRTL</td>
<td>nonrandom two-liquid</td>
</tr>
<tr>
<td>NSOM</td>
<td>near-field scanning optical microscopy</td>
</tr>
<tr>
<td>NTP</td>
<td>normal temperature and pressure</td>
</tr>
<tr>
<td>NTRP</td>
<td>unspecified nucleoside 5′-triphosphate</td>
</tr>
<tr>
<td>Nuc</td>
<td>nucleoside (unspecified)</td>
</tr>
<tr>
<td>Nva</td>
<td>norvalyl, norvaline</td>
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<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
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<tbody>
<tr>
<td>ω</td>
<td>angular frequency</td>
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<tr>
<td>Ω</td>
<td>ohm</td>
</tr>
<tr>
<td>o</td>
<td>ortho</td>
</tr>
<tr>
<td>O</td>
<td>orotidine</td>
</tr>
<tr>
<td>o.d.</td>
<td>outside diameter</td>
</tr>
<tr>
<td>o-rh</td>
<td>orthorhombic (crystal structure)</td>
</tr>
<tr>
<td>o/w</td>
<td>oil in water (emulsion)</td>
</tr>
<tr>
<td>O/W</td>
<td>oil in water (emulsion)</td>
</tr>
<tr>
<td>OAc</td>
<td>acetate</td>
</tr>
<tr>
<td>obsd</td>
<td>observed</td>
</tr>
<tr>
<td>OC-6</td>
<td>octahedral, coordination number 6</td>
</tr>
<tr>
<td>OCR</td>
<td>optical character recognition</td>
</tr>
<tr>
<td>OD</td>
<td>optical density</td>
</tr>
<tr>
<td>ODMR</td>
<td>optically detected magnetic resonance</td>
</tr>
<tr>
<td>ODU</td>
<td>optical density unit</td>
</tr>
<tr>
<td>Oe</td>
<td>oersted</td>
</tr>
<tr>
<td>OES</td>
<td>optical emission spectroscopy</td>
</tr>
<tr>
<td>OFDR</td>
<td>off-frequency decoupling resonance</td>
</tr>
<tr>
<td>OMVPE</td>
<td>organometallic vapor-phase epitaxy</td>
</tr>
<tr>
<td>Ord</td>
<td>orotidine</td>
</tr>
<tr>
<td>ORD</td>
<td>optical rotary dispersion</td>
</tr>
<tr>
<td>Orn</td>
<td>ornithyl, ornithine</td>
</tr>
<tr>
<td>Oro</td>
<td>orotic acid</td>
</tr>
<tr>
<td>ORTEP</td>
<td>Oak Ridge thermal ellipsoid plot</td>
</tr>
<tr>
<td>osm</td>
<td>osmolar (also osM, Osm)</td>
</tr>
<tr>
<td>OTTLE</td>
<td>optically transparent thin-layer electrode</td>
</tr>
<tr>
<td>ox</td>
<td>oxalato (ligand)</td>
</tr>
<tr>
<td>oxidn</td>
<td>oxidized or oxidation (in subscripts and superscripts)</td>
</tr>
<tr>
<td>oz</td>
<td>ounce</td>
</tr>
</tbody>
</table>
% percent
‰ per thousand (parts per thousand)
π pros (near) in NMR measurements (as in N² of histidine)
type of orbital, electron
π⁺ pion
π⁰ pion
ψ pseudouridine
ψrd pseudouridine
p negative logarithm (as in pH)
page
pico (10⁻¹²)
proton
p angular momentum (ESR and NMR spectroscopy)
para
probability (in statistics)
pyranose form
P peta (10¹⁵)
opoise
proline
ρ plus (right-handed helix)
probability (in statistics)
p.m. post meridiem
P450 specific cytochrome designation (i.e., cytochrome P450)
P-450 specific cytochrome designation (i.e., cytochrome P-450)
P₄5₀ specific cytochrome designation (i.e., cytochrome P₄5₀)
³¹P NMR phosphorus-3¹ nuclear magnetic resonance
Pa pascal
PAC perturbed angular correlation
PAD perturbed angular distribution
PAGE polyacrylamide gel electrophoresis
p₄H negative logarithm of hydrogen ion activity
PAH polycyclic aromatic hydrocarbon
PAN polacrylonitrile
PBS phosphate-buffered saline
pc parsec (unit of length)
PC paper chromatography
personal computer
planar chromatography
PCB polychlorobiphenyl, polychlorinated biphenyl
PCDD polychlorinated dibenzo-p-dioxin
PCDF polychlorodibenzo-p-dioxin
polychlorodibenzofuran
PCIILO perturbed configuration interaction with localized orbitals
PCP pentachlorophenol
PCR polymerase chain reaction
PCTFE poly(chlorotrifluoroethylene)
<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Full Form</th>
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<tbody>
<tr>
<td>PDL</td>
<td>pumped dye laser</td>
</tr>
<tr>
<td>PDMS</td>
<td>plasma desorption mass spectrometry</td>
</tr>
<tr>
<td>PE</td>
<td>polyethylene</td>
</tr>
<tr>
<td></td>
<td>potential energy</td>
</tr>
<tr>
<td>PEG</td>
<td>poly(ethylene glycol)</td>
</tr>
<tr>
<td>PEL</td>
<td>permissible exposure limit</td>
</tr>
<tr>
<td>PEO</td>
<td>poly(ethylene oxide)</td>
</tr>
<tr>
<td>PES</td>
<td>photoelectron spectroscopy</td>
</tr>
<tr>
<td>PET</td>
<td>positron emission tomography</td>
</tr>
<tr>
<td>PETP</td>
<td>poly(ethylene terephthalate)</td>
</tr>
<tr>
<td>PFU</td>
<td>plaque-forming unit</td>
</tr>
<tr>
<td>PG</td>
<td>prostaglandin</td>
</tr>
<tr>
<td>pH</td>
<td>negative logarithm of hydrogen ion concentration</td>
</tr>
<tr>
<td>Ph</td>
<td>phenyl (for C$_6$H$_5$ only)</td>
</tr>
<tr>
<td>Phe</td>
<td>phenylalanin, phenylalanine</td>
</tr>
<tr>
<td>phen</td>
<td>1,10-phenanthroline, o-phenanthroline</td>
</tr>
<tr>
<td>phr</td>
<td>parts per hundred parts of resin (or rubber)</td>
</tr>
<tr>
<td>P$_i$</td>
<td>inorganic phosphate</td>
</tr>
<tr>
<td>PIB</td>
<td>polyisobutylene</td>
</tr>
<tr>
<td>PIXE</td>
<td>proton-induced X-ray emission</td>
</tr>
<tr>
<td>pK</td>
<td>negative logarithm of equilibrium constant</td>
</tr>
<tr>
<td>pK$_a$</td>
<td>pK for association</td>
</tr>
<tr>
<td>PL</td>
<td>photoluminescence</td>
</tr>
<tr>
<td>PLOT</td>
<td>porous-layer open-tubular</td>
</tr>
<tr>
<td>PMMA</td>
<td>poly(methyl methacrylate)</td>
</tr>
<tr>
<td>PMO</td>
<td>perturbational molecular orbital</td>
</tr>
<tr>
<td>PMR</td>
<td>phosphorus magnetic resonance (do not use; use $^{31}$P NMR)</td>
</tr>
<tr>
<td></td>
<td>polymerization of monomeric reactants</td>
</tr>
<tr>
<td></td>
<td>proton magnetic resonance (do not use; use $^1$H NMR)</td>
</tr>
<tr>
<td>PNA</td>
<td>polynuclear aromatic hydrocarbon</td>
</tr>
<tr>
<td>PNDO</td>
<td>partial neglect of differential overlap</td>
</tr>
<tr>
<td>po</td>
<td>per os (orally)</td>
</tr>
<tr>
<td>POM</td>
<td>poly(oxyethylene), polyformaldehyde</td>
</tr>
<tr>
<td>POPPOP</td>
<td>1,4-bis(5-phenyl-2-oxazolyl)benzene</td>
</tr>
<tr>
<td>pp</td>
<td>pages</td>
</tr>
<tr>
<td>PP</td>
<td>polypropene</td>
</tr>
<tr>
<td>ppb</td>
<td>parts per billion</td>
</tr>
<tr>
<td>ppbv</td>
<td>parts per billion by volume</td>
</tr>
<tr>
<td>PP$_i$</td>
<td>inorganic pyrophosphate, phosphoric acid</td>
</tr>
<tr>
<td>ppm</td>
<td>parts per million</td>
</tr>
<tr>
<td>ppmv</td>
<td>parts per million by volume</td>
</tr>
<tr>
<td>PPO</td>
<td>2,5-diphenyloxazol</td>
</tr>
<tr>
<td>PPP</td>
<td>Pariser–Parr–Pople</td>
</tr>
<tr>
<td>PPS</td>
<td>photophoretic spectroscopy</td>
</tr>
<tr>
<td>ppt</td>
<td>parts per trillion</td>
</tr>
<tr>
<td></td>
<td>precipitate</td>
</tr>
</tbody>
</table>
pptv  parts per trillion by volume
Pr   propyl
PRDDO partial retention of diatomic differential overlap
prepn preparation
PRFT partially relaxed Fourier transform
Pro  prolyl, proline
pro-R stereochemical descriptor (also pro-R)
pro-S stereochemical descriptor (also pro-S)
PRFT partially relaxed Fourier transform
Ps   positronium
PS   polystyrene
psi  pounds per square inch
psia pounds per square inch absolute
psig pounds per square inch gauge
pt   pint
point
PTC  phase-transfer catalysis
PTFE poly(tetrafluoroethylene)
PTH  parathyroid hormone
phenylthiohydantoin
PTV  programmed-temperature vaporizer
PU   polyurethane
PVA  poly(vinyl alcohol)
PVAC poly(vinyl acetate)
PVAL poly(vinyl alcohol)
PVC  poly(vinyl chloride)
PVDC poly(vinylidene dichloride)
PVDF poly(vinylidene difluoride)
PVE  poly(vinyl ether)
PVF  poly(vinyl fluoride)
PXRD powder X-ray diffraction
py   pyridine (ligand)
Py   pyridine
PY   pyramidal (coordination compounds)
Py–GC–MS pyrolysis–gas chromatography–mass spectrometry
pyr  pyrazine (ligand)
pyrr pyrrolidine (ligand)
pz   pyrazole (ligand)

q    quartet (spectra)
q    heat, electric charge (also Q)
Q    glutamine
Q    heat, electric charge (also q)
QCPE Quantum Chemistry Program Exchange
QELS quasi-elastic light scattering
QSAR quantitative structure–activity relationship
qt   quart
\( \rho \)  
Density

\( r \)  
Correlation coefficient

\( R \)  
Arginine

Rankine (temperature scale, use °R as unit abbreviation)

Roentgen

\( R \)  
Gas constant

Rectus (configurational)

Regression coefficient

Resistance

\( \text{rac} \)  
Racemic

\( \text{rad} \)  
Radian

Unit of radiation

\( \text{RBS} \)  
Rutherford backscattering spectrometry

\( \text{rd} \)  
Rad

\( \text{RDE} \)  
Rotating disk electrode

\( r_e \)  
Electron radius

\( \text{re} \)  
Stereochemical descriptor (as in the re face)

Recryst

Recrystallized

\( \text{red} \)  
Reduced or reduction (in subscripts and superscripts)

\( \text{redn} \)  
Reduction

\( \text{redox} \)  
Reduction–oxidation

\( \text{ref} \)  
Reference

\( \text{rel} \)  
Relative

\( \text{rel} \)  
Relative (stereochemical descriptor)

\( \text{REL} \)  
Recommended exposure limit

\( \text{rem} \)  
Roentgen equivalent man

\( \text{REM} \)  
Rapid eye movement

\( \text{rep} \)  
Roentgen equivalent physical

\( \text{rf} \)  
Radio frequency

\( R_f \)  
Retention factor (ratio of distance traveled by the center of a zone to the distance simultaneously traveled by the mobile phase)

\( \text{RFC} \)  
Request for comments

\( \text{RH} \)  
Relative humidity

\( \text{Rha} \)  
Rhamnose

\( \text{RI} \)  
Refractive index

\( \text{RIA} \)  
Radioimmunoassay

\( \text{Rib} \)  
Ribose

\( \text{RIMS} \)  
Resonance ionization mass spectrometry

\( \text{RIS} \)  
Resonance ionization spectrometry

\( \text{rms} \)  
Root mean square

\( \text{RNA} \)  
Ribonucleic acid

\( \text{RNase} \)  
Ribonuclease

\( \text{ROA} \)  
Raman optical activity

\( \text{RPLC} \)  
Reversed-phase liquid chromatography

\( \text{rpm} \)  
Revolutions per minute

\( \text{RQ} \)  
Respiratory quotient

\( \text{RRDE} \)  
Rotating ring-disk electrode
RRKM Rice–Ramsperger–Kassel–Marcus
rRNA ribosomal RNA
RRS resonance Raman spectroscopy
RRT relative retention time
RS Raman spectroscopy
RSD relative standard deviation
risk-specific dose
Ry rydberg

σ standard deviation
surface charge density
surface tension
tensile strength
type of orbital, electron
Σ summation
s second
single bond [as in s-cis (italic in compound names)]
singlet (spectra)
solid [as in NaCl(s)]
strong (spectra)
s secondary (as in s-Bu; but sec-butyl)
sedimentation coefficient
standard deviation (analytical)
symmetrical

\( s_{20,w} \) sedimentation coefficient measured at 20 °C in water and extrapolated to 0 °C

\( s^2 \) sample variance
S serine
siemens
S entropy
sinister (configurational)
skew (conformation)
S/N signal-to-noise ratio
SAM self-assembled monolayer
SANS small-angle neutron scattering
SAPR-8 square antiprismatic, coordination number 8
sar sarcosine (\( N \)-methylglycine) (ligand)
Sar sarcosyl, sarcosine (\( N \)-methylglycine)
SAR structure–activity relationship
SARISA surface analysis by resonance ionization of sputtered atoms
SAXS small-angle X-ray scattering (or spectroscopy)
sc subcutaneously
sc synclinal
scem standard cubic centimeters per minute
SCE saturated calomel electrode
SCF self-consistent field
SCF–HF self-consistent field, Hartree–Fock
<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
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</thead>
<tbody>
<tr>
<td>scfh</td>
<td>standard cubic feet per hour</td>
</tr>
<tr>
<td>SCOT</td>
<td>support-coated open-tubular</td>
</tr>
<tr>
<td>SD</td>
<td>standard deviation</td>
</tr>
<tr>
<td>SDS</td>
<td>sodium dodecyl sulfate</td>
</tr>
<tr>
<td>SE</td>
<td>standard error</td>
</tr>
<tr>
<td>S&lt;sub&gt;2&lt;/sub&gt;</td>
<td>second-order electrophilic substitution</td>
</tr>
<tr>
<td>sec</td>
<td>secant</td>
</tr>
<tr>
<td>sec</td>
<td>secondary (as in sec-butyl; but s-Bu)</td>
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<tr>
<td>SEC</td>
<td>size exclusion chromatography</td>
</tr>
<tr>
<td>sech</td>
<td>hyperbolic secant</td>
</tr>
<tr>
<td>SECM</td>
<td>scanning electrochemical microscopy</td>
</tr>
<tr>
<td>SECS</td>
<td>simulation and evaluation of chemical synthesis</td>
</tr>
<tr>
<td>SEM</td>
<td>scanning electron microscopy</td>
</tr>
<tr>
<td>Ser</td>
<td>seryl, serine</td>
</tr>
<tr>
<td>SERS</td>
<td>surface-enhanced Raman spectroscopy (or scattering)</td>
</tr>
<tr>
<td>SEW</td>
<td>surface electromagnetic wave</td>
</tr>
<tr>
<td>S&lt;sub&gt;ex&lt;/sub&gt;</td>
<td>exciplex substitution</td>
</tr>
<tr>
<td>SFC</td>
<td>supercritical-fluid chromatography</td>
</tr>
<tr>
<td>sh</td>
<td>sharp (spectra)</td>
</tr>
<tr>
<td>Sh</td>
<td>Sherwood number</td>
</tr>
<tr>
<td>SHC</td>
<td>shape and Hamiltonian constant</td>
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<tr>
<td>SHE</td>
<td>standard hydrogen electrode</td>
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<tr>
<td>si</td>
<td>stereochemical descriptor (as in the si face)</td>
</tr>
<tr>
<td>SI</td>
<td>International System of Units (Système International)</td>
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<tr>
<td>SIM</td>
<td>selected-ion monitoring</td>
</tr>
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<td>SIMS</td>
<td>secondary-ion mass spectrometry</td>
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<tr>
<td>sin</td>
<td>sine</td>
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<tr>
<td>sinh</td>
<td>hyperbolic sine</td>
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<tr>
<td>SLR</td>
<td>spin–lattice relaxation</td>
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<td>SMOSS</td>
<td>surface Mössbauer</td>
</tr>
<tr>
<td>SMSI</td>
<td>strong metal support interaction</td>
</tr>
<tr>
<td>sn</td>
<td>stereospecific numbering</td>
</tr>
<tr>
<td>SN</td>
<td>separation number</td>
</tr>
<tr>
<td>S&lt;sub&gt;N&lt;/sub&gt;1</td>
<td>first-order nucleophilic substitution</td>
</tr>
<tr>
<td>S&lt;sub&gt;N&lt;/sub&gt;2</td>
<td>second-order nucleophilic substitution</td>
</tr>
<tr>
<td>S&lt;sub&gt;N&lt;/sub&gt;i</td>
<td>internal nucleophilic substitution</td>
</tr>
<tr>
<td>SNO</td>
<td>semiempirical natural orbital</td>
</tr>
<tr>
<td>sol</td>
<td>solid</td>
</tr>
<tr>
<td>soln</td>
<td>solution</td>
</tr>
<tr>
<td>sp</td>
<td>specific</td>
</tr>
<tr>
<td>sp.</td>
<td>species (singular)</td>
</tr>
<tr>
<td>sp</td>
<td>synperiplanar</td>
</tr>
<tr>
<td>SP-4</td>
<td>square planar, coordination number 4</td>
</tr>
<tr>
<td>sp gr</td>
<td>specific gravity</td>
</tr>
</tbody>
</table>
sp ht specific heat
sp vol specific volume
SPECT single-photon-emission computed tomography
spp. species (plural)
SPR stroboscopic pulse radiolysis
SPY-5 square pyramidal, coordination number 5
sq square
SQF single quantum filtered
SQUID superconducting quantum interference device
sr steradian
S_{RN}^{1} first-order nucleophilic substitution triggered by electron transfer
SRS stimulated Raman scattering
SSC standard saline citrate (NaCl–citrate)
St stokes
std standard
STEM scanning transmission electron microscopy
STM scanning tunneling microscopy
STO Slater-type orbital
STO-3G Slater-type orbital, three Gaussian
STP standard temperature and pressure
subsp. subspecies
Suc sucrose
Sv sievert
sv svedberg
SVL single vibrational level
swg standard wire gauge
sym symmetrical

τ tele (far) in NMR measurements (as in N\textsuperscript{τ} of histidine)
θ angle
[θ] ORD measurement, deg cm\textsuperscript{2}/dmol
Θ temperature (e.g., in Curie–Weiss expressions)
t metric ton
triplet (spectra)
triton

\( t \) Student distribution (the Student \( t \) test in statistics)
temperature (in degrees Celsius)
tertiary (as in \( t \)-Bu; but \( tert \)-butyl)
time
\( t_{1/2} \) half-life
T ribosylthymine
tautomeric
tera (10\textsuperscript{12})
tesla
threonine
tritium
<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T$</td>
<td>temperature (in kelvins)</td>
</tr>
<tr>
<td>$T$-4</td>
<td>tetrahedral, coordination number 4</td>
</tr>
<tr>
<td>T/C</td>
<td>treated vs cured</td>
</tr>
<tr>
<td>tan</td>
<td>tangent</td>
</tr>
<tr>
<td>tan $\delta$</td>
<td>mechanical loss factor</td>
</tr>
<tr>
<td>tanh</td>
<td>hyperbolic tangent</td>
</tr>
<tr>
<td>TBP</td>
<td>tri-$n$-butyl phosphate</td>
</tr>
<tr>
<td>TBPY-5</td>
<td>trigonal bipyramidal, coordination number 5</td>
</tr>
<tr>
<td>TCA</td>
<td>tricarboxylic acid cycle (citric acid cycle, Krebs cycle)</td>
</tr>
<tr>
<td>TCD</td>
<td>thermal conductivity detector</td>
</tr>
<tr>
<td>TCP/IP</td>
<td>transmission control protocol/Internet protocol</td>
</tr>
<tr>
<td>TDS</td>
<td>total dissolved solids</td>
</tr>
<tr>
<td>TEA</td>
<td>tetraethylammonium</td>
</tr>
<tr>
<td>TEAE</td>
<td>transversely excited atmospheric</td>
</tr>
<tr>
<td>TEM</td>
<td>transmission electron microscopy</td>
</tr>
<tr>
<td>temp</td>
<td>temperature</td>
</tr>
<tr>
<td>tert</td>
<td>tertiary (as in tert-butyl; but $t$-Bu)</td>
</tr>
<tr>
<td>tetr</td>
<td>tetragonal (crystal structure)</td>
</tr>
<tr>
<td>TFA</td>
<td>trifluoroacetyl</td>
</tr>
<tr>
<td>$T_g$</td>
<td>glass-transition temperature</td>
</tr>
<tr>
<td>TGA</td>
<td>thermogravimetric analysis</td>
</tr>
<tr>
<td>Tham</td>
<td>tris(hydroxymethyl)aminomethane (also Tris)</td>
</tr>
<tr>
<td>THC</td>
<td>tetrahydrocannabinol</td>
</tr>
<tr>
<td>Thd</td>
<td>ribosylthymine</td>
</tr>
<tr>
<td>theor</td>
<td>theoretical</td>
</tr>
<tr>
<td>THF</td>
<td>tetrahydrofuran</td>
</tr>
<tr>
<td>Thr</td>
<td>threonyl, threonine</td>
</tr>
<tr>
<td>Thy</td>
<td>thymine</td>
</tr>
<tr>
<td>TIMS</td>
<td>thermal ionization mass spectrometry</td>
</tr>
<tr>
<td>TIP</td>
<td>temperature-independent paramagnetism</td>
</tr>
<tr>
<td>TL</td>
<td>triboluminescence</td>
</tr>
<tr>
<td>TLC</td>
<td>thin-layer chromatography</td>
</tr>
<tr>
<td>TMA</td>
<td>thermomechanical analysis</td>
</tr>
<tr>
<td>TMS</td>
<td>tetramethysilane</td>
</tr>
<tr>
<td>TMV</td>
<td>tobacco mosaic virus</td>
</tr>
<tr>
<td>TnL</td>
<td>tunnel luminescence</td>
</tr>
<tr>
<td>TOC</td>
<td>total organic carbon</td>
</tr>
<tr>
<td>TOD</td>
<td>total oxygen demand</td>
</tr>
<tr>
<td>TOFMS</td>
<td>time-of-flight mass spectrometry (also TOF MS)</td>
</tr>
<tr>
<td>tol</td>
<td>tolyl (also Tol)</td>
</tr>
<tr>
<td>TOM</td>
<td>transmitted optical microscopy</td>
</tr>
<tr>
<td>Torr</td>
<td>torr</td>
</tr>
<tr>
<td>Abbreviation</td>
<td>Description</td>
</tr>
<tr>
<td>--------------</td>
<td>-------------</td>
</tr>
<tr>
<td>tosyl</td>
<td>4-toluenesulfonyl (also Ts)</td>
</tr>
<tr>
<td>TPD</td>
<td>temperature-programmed desorption</td>
</tr>
<tr>
<td>TPDE</td>
<td>temperature-programmed decomposition</td>
</tr>
<tr>
<td>TPR</td>
<td>temperature-programmed reduction</td>
</tr>
<tr>
<td>TPR-6</td>
<td>trigonal prismatic, coordination number 6</td>
</tr>
<tr>
<td>TQMS</td>
<td>triple-quadrupole mass spectrometry</td>
</tr>
<tr>
<td>( t_R )</td>
<td>retention time</td>
</tr>
<tr>
<td>tr</td>
<td>trace</td>
</tr>
<tr>
<td>Tr</td>
<td>trace</td>
</tr>
<tr>
<td>tric</td>
<td>triclinic (crystal structure)</td>
</tr>
<tr>
<td>triflate</td>
<td>trifluoromethanesulfonate</td>
</tr>
<tr>
<td>trig</td>
<td>trigonal (crystal structure)</td>
</tr>
<tr>
<td>TRIR</td>
<td>time-resolved infrared</td>
</tr>
<tr>
<td>Tris</td>
<td>tris(hydroxymethyl)aminomethane (also Tham)</td>
</tr>
<tr>
<td>tRNA</td>
<td>transfer RNA</td>
</tr>
<tr>
<td>Trp</td>
<td>tryptophyl, tryptophan</td>
</tr>
<tr>
<td>Ts</td>
<td>tosyl (4-toluenesulfonyl)</td>
</tr>
<tr>
<td>TSC</td>
<td>thermal stimulated current</td>
</tr>
<tr>
<td>TSH</td>
<td>thyroid-stimulating hormone</td>
</tr>
<tr>
<td>tu</td>
<td>thiourea (ligand)</td>
</tr>
<tr>
<td>TVA</td>
<td>thermal volatilization analysis</td>
</tr>
<tr>
<td>Tyr</td>
<td>tyrosyl, tyrosine</td>
</tr>
<tr>
<td>u</td>
<td>unified atomic mass unit</td>
</tr>
<tr>
<td>U</td>
<td>uniformly labeled</td>
</tr>
<tr>
<td>( U )</td>
<td>internal energy</td>
</tr>
<tr>
<td>uridine</td>
<td>uridine</td>
</tr>
<tr>
<td>UCST</td>
<td>upper critical solution temperature</td>
</tr>
<tr>
<td>UDP</td>
<td>uridine 5’-diphosphate</td>
</tr>
<tr>
<td>uhf</td>
<td>ultrahigh frequency</td>
</tr>
<tr>
<td>UHF</td>
<td>ultrahigh frequency</td>
</tr>
<tr>
<td>unrestricted Hartree–Fock</td>
<td></td>
</tr>
<tr>
<td>UHV</td>
<td>ultrahigh vacuum</td>
</tr>
<tr>
<td>ULSI</td>
<td>ultra-large-scale integration</td>
</tr>
<tr>
<td>UMP</td>
<td>uridine 5’-monophosphate, uridine 5’-phosphate</td>
</tr>
<tr>
<td>uncor</td>
<td>uncorrected</td>
</tr>
<tr>
<td>uns</td>
<td>unsymmetrical</td>
</tr>
<tr>
<td>UPS</td>
<td>ultraviolet photoelectron spectroscopy</td>
</tr>
<tr>
<td>ur</td>
<td>urea (ligand)</td>
</tr>
<tr>
<td>Ura</td>
<td>uracil</td>
</tr>
<tr>
<td>Urd</td>
<td>uridine</td>
</tr>
<tr>
<td>USP</td>
<td>United States Pharmacopeial Convention</td>
</tr>
<tr>
<td>UTP</td>
<td>uridine 5’-triphosphate</td>
</tr>
<tr>
<td>UV</td>
<td>ultraviolet</td>
</tr>
<tr>
<td>UV PES</td>
<td>ultraviolet photoelectron spectroscopy</td>
</tr>
<tr>
<td>UV–vis</td>
<td>ultraviolet–visible</td>
</tr>
</tbody>
</table>
v  vendeko (10^{-30})
v  scan rate
velocity
V  valine
vendeca (10^{30})
volt
v/v  volume per volume
Val  valyl, valine
VASS  variable-angle sample spinning
VB  valence bond
VCD  vibrational circular dichroism
VDT  video display terminal
VEELS  vibrational electron energy loss spectroscopy
VESCF  variable electronegativity self-consistent field
vhf  very high frequency
VHF  very high frequency
vic  vicinal
vis  visible
viz.  namely
VLE  vapor–liquid equilibrium
VLSI  very large scale integration
VOA  vibrational optical activity
VOC  volatile organic compound
vol  volume
vol %  volume percent
vp  vapor pressure
VPC  vapor-phase chromatography
VPO  vapor pressure osmometry
VRML  virtual reality modeling language
vs  versus (v in legal expressions)
  very strong (spectra)
VSIP  valence-state ionization potential
VUV  vacuum ultraviolet
VVk  Van Vleck
vw  very weak (spectra)

w  weak (spectra)
\textit{w}  weighting factor
  work
W  tryptophan
  watt
\emph{W}  work
w/v  weight per volume
w/w  weight per weight
WAN  wide-area network
WAXS  wide-angle X-ray scattering
Wb  weber
WCOT  wall-coated open-tubular
WDS  wavelength-dispersive spectroscopy
WHSV  weight-hourly space velocity
WLF  Williams–Landel–Ferry (molecular models)
wt  weight
wt %  weight percent

x  xenno \(10^{-27}\)
x  x axis
X  xanthosine (use N for unknown nucleoside)
xenna \(10^{27}\)
Xan  xanthine
XANES  X-ray absorption near-edge spectroscopy
X-ray absorption near-edge structure
Xao  xanthosine
XEDS  X-ray energy-dispersive spectrometry
XES  X-ray emission spectroscopy
XMP  xanthosine 5‘-monophosphate, xanthosine 5‘-phosphate
XPS  X-ray photoelectron spectroscopy
XRD  X-ray diffraction
XRDF  X-ray radial distance function
XRF  X-ray fluorescence
Xyl  xylose

y  yocto \(10^{-24}\)
y  y axis
Y  tyrosine
yotta \(10^{24}\)

z  zepto \(10^{-21}\)
z  charge number of an ion
z axis
Z  benzyloxycarbonyl (also Cbz)
“glutamic acid or glutamine”
zetta \(10^{21}\)
Z  atomic number
zusammen (configurational)
zfs  zero-field splitting
zfsc  zero-field-splitting constant
CHAPTER 11

Numbers, Mathematics, and Units of Measure

Numbers

Both numerals and words can be used to express numbers. The usage and style conventions for numerals and words are different for technical and nontechnical material.

Numeral and Word Usage

➤ Use numerals with units of time or measure, and use a space between the numeral and the unit, except %, $, ° (angular degrees), ′ (angular minutes), and ″ (angular seconds).

<table>
<thead>
<tr>
<th>6 min</th>
<th>25 mL</th>
<th>125 V/s</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.30 g</td>
<td>50%</td>
<td>$250</td>
</tr>
<tr>
<td>273 K</td>
<td>47°8′23″</td>
<td>180° (but 180 °C)</td>
</tr>
<tr>
<td>90 °F</td>
<td>50 µg of compound/dL of water</td>
<td></td>
</tr>
</tbody>
</table>

EXCEPTION Spell out numbers with units of measure used in a nontechnical sense.

If you take five minutes to read this article, you’ll be surprised.

➤ With items other than units of time or measure, use words for cardinal numbers less than 10; use numerals for 10 and above. Spell out ordinals “first” through “ninth”; use numerals for 10th or greater.

three flasks 30 flasks
The ACS Style Guide

third flask 12th flask
seven trees 10 trees
eighth example 33rd example
first century 21st century
sixfold 20-fold

Exception 1 Use all numerals in a series or range containing numbers 10 or greater, even in nontechnical text.

5, 8, and 12 experiments
2nd and 20th samples
5–15 repetitions

Exception 2 Use all numerals for numbers modifying nouns in parallel construction in the same sentence if one of the numbers is 10 or greater.

Activity was reduced in 2 pairs, not significantly changed in 11 pairs, and increased in 6 pairs.

We present new results pertaining to 12 phenanthrolines and 3 porphyrins.

Exception 3 For very large numbers used in a nontechnical sense, use a combination of numerals and words.

1 billion tons
180 million people
2 million pounds (not lb)
4.5 billion years
$15 million (not 15 million dollars)

► When a sentence starts with a specific quantity, spell out the number as well as the unit of measure.

Twelve species were evaluated in this study.
Twenty slides of each blood sample were prepared.
Fifteen milliliters of supernate was added to the reaction vessel.
Twenty-five milliliters of acetone was added, and the mixture was centrifuged.

However, if possible, recast the sentence.

Acetone (25 mL) was added, and the mixture was centrifuged.
A 25 mL portion of acetone was added, and the mixture was centrifuged.

► Even when a sentence starts with a spelled-out quantity, use numerals when appropriate in the rest of the sentence.

Twenty-five milliliters of acetone and 5 mL of HCl were added.
Three micrograms of sample was dissolved in 20 mL of acid.
Fifty samples were collected, but only 22 were tested.
➤ Use numerals for expressions used in a mathematical sense.

The incidence of disease increased by a factor of 4.
The yield of product was decreased by 6 orders of magnitude.
The efficiency of the reaction was increased 2-fold.
After 2 half-lives, the daughter product could be measured.
The control group had 3 times the risk for colon cancer.
The values are determined with 5 degrees of freedom.

➤ When the suffix “fold” is used in a nonmathematical sense, spell out the accompanying number if it is less than 10.

The purpose of this discussion is twofold.

➤ When the word “times” is used in a nonmathematical sense, spell out the accompanying number if it is less than 10.

The beaker was rinsed four times.

➤ Use numerals in ratios.

a ratio of 1:10
a ratio of 1/10
a 1:1 (v/v) mixture
a 1/1 (v/v) mixture

➤ In dates, use numerals without ordinal endings.

January 3, Jan 3 (not January 3rd, Jan 3rd)
September 5, Sept 5 (not September 5th, Sept 5th)

➤ Use numerals for decades, and form their plurals by adding an “s”. Do not use apostrophes in any position.

the 1960s (not the 1960’s, not the ’60s)
values in the 90s (not the 90’s)
She is in her 20s. (not her 20’s)

➤ Use numerals with a.m. and p.m.

12:15 a.m.  4:00 p.m.

➤ Spell out and hyphenate fractions whose terms are both less than 10. If one of the terms is 10 or greater, use a piece fraction.

one-quarter of the experiments  \( \frac{1}{4} \) of the subjects
two-thirds of the results  \( \frac{2}{3} \) of the volume
Use numerals to label figures, tables, schemes, structures, charts, equations, and references. Number sequentially; do not skip numbers or number out of sequence. Use arabic numerals for references, but for the other items, the use of arabic and roman numerals varies among ACS publications. Consult a recent issue or author instructions to determine what system is preferred.

In journal articles and book chapters, instead of repeating chemical names over and over, use numerals in boldface (not italic) type to identify chemical species. Use these identifiers only in text, not in article or chapter titles, and number consecutively.

This paper describes the syntheses, structures, and stereodynamic behavior of the novel hexacoordinate silicon complexes 1–4.

The cyclization of 1,3,5-hexatriene (6) to 1,3-cyclohexadiene (7) is predicted to proceed more rapidly in an electrostatic field.

Complexes 8–12, in the presence of monoamine oxidase, produce active catalysts for propylene polymerization.

Primary amines 2–5, 7, and 9 gave the same Cotton effect signs, depending on the configuration.

Monomer III reacts with the initiator (I, Ar = 2,6-diisopropylphenyl) via a ring-opening metathesis polymerization mechanism.

Numerals may be used to name members of a series.

Sample 1 contained a high level of contamination, but samples 2 and 3 were relatively pure.

Methods 1 and 2 were used for water-soluble compounds, and methods 3 and 4 were used for oil-soluble compounds.

When numerals are used as names and not enumerators, form their plurals by adding an apostrophe and “s” to avoid confusion with mathematical expressions and to make it clear that the “s” is not part of the name.

The athlete received five 9’s from the judges.

Boeing 747’s are among the largest airplanes.

Arabic numerals in parentheses may be used to enumerate a list of phrases or sentences in text. Always use an opening and a closing parenthesis, not one alone.

Some advantages of these materials are (1) their electrical properties after pyrolysis, (2) their ability to be modified chemically before pyrolysis, and (3) their abundance and low cost.

The major conclusions are the following: (1) We have further validated the utility of molecular mechanical methods in simulating the kinetics of these reactions.
(2) A comparison of the calculated structures with available X-ray structures revealed satisfactory agreement. (3) The combined use of different theoretical approaches permitted characterization of the properties of a new isomer.

➤ Arabic numerals followed by periods or enclosed in parentheses may be used to enumerate a displayed list of sentences or to number paragraphs. Here are two acceptable ways to format a list.

These results suggest the following:
1. Ketones are more acidic than esters.
2. Cyclic carboxylic acids are more acidic than their acyclic analogues.
3. Alkylation of the active methylene carbon reduces the acidity.

These results suggest the following:
(1) Ketones are more acidic than esters.
(2) Cyclic carboxylic acids are more acidic than their acyclic analogues.
(3) Alkylation of the active methylene carbon reduces the acidity.

**Style for Numbers**

➤ For very large numbers with units of measure, use scientific notation or choose an appropriate multiplying prefix for the unit to avoid numbers of more than four digits.

- $1.2 \times 10^6 \text{ s}$
- $3.0 \times 10^4 \text{ kg}$
- $5.8 \times 10^{-5} \text{ M or 58 \mu M}$
- $42.3 \text{ L (not 42,300 mL or 42 300 mL)}$

**EXCEPTION 1** In tables, use the same unit and multiplying prefix for all entries in a column, even if some entries therefore require four or more digits.

**EXCEPTION 2** Use the preferred unit of a discipline, even when the numbers require four or more digits:

- $\text{g/L}$ for mass density of fluids
- $\text{kg/m}^3$ for mass density of solids
- $\text{GPa}$ for modulus of elasticity
- $\text{kPa}$ for fluid pressure
- $\text{MPa}$ for stress

➤ In four-digit numbers, use no commas or spaces.

**EXCEPTION** Spaces or commas are inserted in four-digit numbers when alignment is needed in a column containing numbers of five or more digits.

➤ When a long number cannot be written in scientific notation, the digits must be grouped. For grouping of digits in long numbers (five digits or greater), check the publication in which the manuscript will appear. Two styles are possible.
STYLE 1 In some publications, for numbers with five or more digits, the digits are grouped with commas placed between groups of three counting to the left of the decimal point.

- 4837
- 10,000
- 930,582
- 6,398,210
- 85,798.62578

STYLE 2 In some publications (including ACS journals), for numbers with five or more digits, the digits are grouped with a thin space between groups of three, counting both to the left and to the right of the decimal point.

- 9319.4
- 74 183.0629
- 0.508 27
- 501 736.293 810 4

EXCEPTIONS

- U.S. monetary values are always written with commas: $5,000.
- U.S. patent numbers are always written with commas: U.S. Patent 6,555,655. The patent numbers of other countries should be presented as on the original patent document.
- Page numbers in reference citations are always printed solid: p 11597.

➤ Use the period as the decimal point, never a comma.

➤ Use numerals before and after a decimal point.

- 0.25 (*not*.25)
- 78.0 or 78 (*not*.78.)

➤ Use a decimal and a zero following a numeral only when such usage truly represents the precision of the measurement: 27.0 °C and 27 °C are not interchangeable.

➤ Use decimals rather than fractions with units of time or measure, except when doing so would imply an unwarranted accuracy.

- 3.5 h (*not* 3½ h)
- 5.25 g (*not* 5¼ g)

➤ Standard deviation, standard error, or degree of accuracy can be given in two ways:

- with only the deviation in the least significant digit(s) placed in parentheses following the main number and closed up to it or
- with all digits preceded by a ± and following the main number. Spaces are left on each side of the ±.
2.0089(1) means 2.0089 ± 0.0001
1.4793(23) means 1.4793 ± 0.0023

The shorter version is better in tables. Always specify which measure (e.g., standard deviation or standard error) of uncertainty is being used.

➤ When two numbered items are cited in narrative, use “and”.

Figures 1 and 2
refs 23 and 24
compounds I and II

➤ Use a comma between two reference callouts in parentheses or as superscripts.

Lewis (12, 13) found
Lewis\textsuperscript{12,13} found

When the reference numbers are on the line, the comma is followed by a space; when the numbers are superscripts, the comma is not followed by a space.

➤ Use an en dash in ranges or series of three or more numbered items, whether on the line or in a superscript.

43–49
325–372
2005–2008
Tables 1–4
ref s 3–5

temperatures of 100–125 °C
past results (27–31)

aliquots of 50–100 mL
eqs 6–9
samples 5–10
past results\textsuperscript{27–31}

pp 165–172

exception 1 Do not use an en dash in expressions with the words “from … to” or “between … and”.

from 20 to 80 (not from 20–80)
between 50 and 100 mL (not between 50–100 mL)

exception 2 When either one or both numbers are negative or include a symbol that modifies the number, use the word “to” or “through”, not the en dash.

–20 to +120 K
–145 to –30 °C
≈50 to 60
10 to >600 mL
<5 to 15 mg

➤ For ranges in scientific notation, retain all parts of all numbers or avoid ambiguity by use of parentheses or other enclosing marks.

\(9.2 \times 10^{-3}\) to \(12.6 \times 10^{-3}\) or \((9.2–12.6) \times 10^{-3}\) (not 9.2 to 12.6 \(\times 10^{-3}\))
For very large numbers in ranges, retain all parts of all numbers.

26 million to 35 million

Do not use e or E to mean “multiplied by the power of 10”.

3.7 × 10^5 (not 3.7e5, 3.7E+5)

**Mathematics**

**Mathematical Concepts**

**Variable** A variable is a quantity that changes in value, substance, or amount, such as \( V \) for volume, \( m \) for mass, and \( t \) for time.

**Constant** A constant is a quantity that has a fixed value, such as \( h \) for the Planck constant and \( F \) for the Faraday constant.

**Function** The function \( f(x) = y \) represents a rule that assigns a unique value of \( y \) to every \( x \). The *argument* of the function is \( x \).

**Operator** An operator is a symbol, such as a function (\( d \), derivative; \( \ln \), natural logarithm; and \( \mathcal{H} \), the Hamiltonian operator) or an arithmetic sign (+, –, =, ÷, and \( \times \)), denoting an operation to be performed.

**Physical Quantity** A physical quantity is a product of a numerical value (a pure number) and a unit. Physical quantities may be scalars or vectors, variables or constants.

**Scalar** A scalar is an ordinary number without direction, such as length, temperature, or mass. Any quantity that is not a vector quantity is a scalar quantity.

**Vector** A vector is a quantity with both magnitude and direction, such as force or velocity. For the vector \( \mathbf{V} = [a, b] \) (also denoted as \( \mathbf{V} = [a, b] \)), \( a \) and \( b \) are the *components* of the vector.

**Tensor** A tensor represents a generalized vector with more than two components.

**Matrix** A matrix is represented by a rectangular array of *elements*; an *array* consists of rows and columns. The elements of matrix \( \mathbf{U} \) are \( u_{11}, u_{12}, \text{ etc.} \)

\[
\mathbf{U} = \begin{bmatrix}
  u_{11} & \cdots & u_{1n} \\
  \vdots & \ddots & \vdots \\
  u_{n1} & \cdots & u_{nn}
\end{bmatrix}
\]
**Determinant** The determinant of a matrix is a function that assigns a number to a matrix. For example, the determinant of the $n \times n$ matrix $B$ is represented by

$$\text{det} B = \begin{vmatrix} b_{11} & \cdots & b_{1n} \\ \vdots & \ddots & \vdots \\ b_{n1} & \cdots & b_{nn} \end{vmatrix}$$

**Index** An index is a subscript or superscript character in an element of a matrix, vector, or tensor; indices usually represent numbers. For example, $i$ and $j$ are indices in $b_{ij}$.

Do not confuse abbreviations and mathematical symbols. An abbreviation is usually two or more letters; a mathematical symbol is generally only one letter, possibly with a subscript or superscript. An abbreviation is used in narrative text but seldom appears in equations; a mathematical symbol is preferred in equations and may also be used in text. For example, in text with no equations, PE for potential energy is acceptable, but in mathematical text and equations, $E_p$ is preferred.

**Usage and Style for Symbols**

- Define all symbols for mathematical constants, variables, and unknown quantities the first time you use them in the text. If you use them in the abstract, define them there and then again at their first appearance in text. Do not define standard mathematical constants such as $\pi$, $i$, and $e$.

- Form the plurals of mathematical symbols by adding an apostrophe and “s” if you cannot use a word such as “values” or “levels”.

  large $r$ values is better than large $r$’s

- Do not use an equal sign as an abbreviation for the word “is” or the word “equals” in narrative text.

  $PV = nRT$, where $P$ is pressure (*not* where $P = \text{pressure}$)

  when the temperature is 50 °C (*not* when the temperature = 50 °C)

- Do not use a plus sign as an abbreviation for the word “and” in narrative text.

  a mixture of $A$ and $B$ (*not* a mixture of $A + B$)

- Do not use an asterisk to indicate multiplication except in computer language expressions.
Italic Type

➤ Use italic type for

• variables: $T$ for temperature, $x$ for mole fraction, $r$ for rate
• axes: the $y$ axis
• planes: plane $P$
• components of vectors and tensors: $a_1 + b_1$
• elements of determinants and matrices: $g_n$
• constants: $k_B$, the Boltzmann constant; $g$, the acceleration due to gravity
• functions that describe variables: $f(x)$

➤ Even when you use mathematical constants, variables, and unknown quantities in adjective combinations, retain the italic type.

In this equation, $V_i$ is the frequency of the $i$th mode.

In eq 4, $n$ is the number of extractions and $M$ is the mass remaining after the $n$th extraction.

➤ Use italic type for two-letter variables defining transport properties.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Name</th>
<th>Symbol</th>
<th>Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Al$</td>
<td>Alfvén number</td>
<td>$Ma$</td>
<td>Mach number</td>
</tr>
<tr>
<td>$Bi$</td>
<td>Biot number</td>
<td>$Nu$</td>
<td>Nusselt number</td>
</tr>
<tr>
<td>$Co$</td>
<td>Cowling number</td>
<td>$Pe$</td>
<td>Péclet number</td>
</tr>
<tr>
<td>$Da$</td>
<td>Damkohler number</td>
<td>$Pr$</td>
<td>Prandtl number</td>
</tr>
<tr>
<td>$Eu$</td>
<td>Euler number</td>
<td>$Ra$</td>
<td>Rayleigh number</td>
</tr>
<tr>
<td>$Fo$</td>
<td>Fourier number</td>
<td>$Re$</td>
<td>Reynolds number</td>
</tr>
<tr>
<td>$Fr$</td>
<td>Froude number</td>
<td>$Sc$</td>
<td>Schmidt number</td>
</tr>
<tr>
<td>$Ga$</td>
<td>Galileo number</td>
<td>$Sh$</td>
<td>Sherwood number</td>
</tr>
<tr>
<td>$Gr$</td>
<td>Grashof number</td>
<td>$Sr$</td>
<td>Strouhal number</td>
</tr>
<tr>
<td>$Ha$</td>
<td>Hartmann number</td>
<td>$St$</td>
<td>Stanton number</td>
</tr>
<tr>
<td>$Kn$</td>
<td>Knudsen number</td>
<td>$We$</td>
<td>Weber number</td>
</tr>
<tr>
<td>$Le$</td>
<td>Lewis number</td>
<td>$Wi$</td>
<td>Weissenberg number</td>
</tr>
</tbody>
</table>

Roman Type

➤ Use roman type for

• numerals;
• punctuation and enclosing marks such as square brackets, parentheses, and braces;
• most operators;
• units of measure and time: mg, milligram; K, kelvin; Pa, pascal; mmHg, millimeters of mercury;
• nonmathematical quantities or symbols: R, radical in chemical nomenclature; $S_1$, molecular state; s, atomic orbital;
• multiple-letter abbreviations for variables: IP, ionization potential; cmc, critical micelle concentration;
• mathematical constants:
  - e, the base of the natural logarithm, 2.71828…
  - i, the imaginary number, (−1)\(^{1/2}\)
  - π, 3.14159…
• transposes of matrices: \(A^T\) (\(T\) is the transpose of matrix \(A\));
• points and lines: point \(A\), line \(AB\);
• determinants: \(\det A\) is the determinant of matrix \(A\); and
• trigonometric and other functions:
  - adjoint
  - Airy function
  - argument
  - bound
  - cokernel
  - cosine
  - hyperbolic cosine
  - cotangent
  - hyperbolic cotangent
  - cosecant
  - hyperbolic cosecant
  - determinant
  - dimension
  - divergence
  - error function
  - complement of error function
  - exponential
  - general linear
  - greater lower bound
  - gradient
  - homology
  - imaginary
  - inferior
  - interior
  - kernel

  - \(\lim\)
  - \(\lim \inf\)
  - \(\lim \sup\)
  - \(\ln\)
  - \(\log\)
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**Boldface Type**

- Use boldface type for
  • vectors;
  • tensors;
  • matrices; and
  • multidimensional physical quantities: \(H\), magnetic field strength.
Greek Letters

Greek letters (lightface or boldface) can be used for variables, constants, and vectors and anywhere a Latin letter can be used.

<table>
<thead>
<tr>
<th>NAME</th>
<th>UPPERCASE</th>
<th>LOWERCASE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alpha</td>
<td>Α</td>
<td>α</td>
</tr>
<tr>
<td>Beta</td>
<td>Β</td>
<td>β</td>
</tr>
<tr>
<td>Gamma</td>
<td>Γ</td>
<td>γ</td>
</tr>
<tr>
<td>Delta</td>
<td>Δ</td>
<td>δ, ð</td>
</tr>
<tr>
<td>Epsilon</td>
<td>Е</td>
<td>ε, ë</td>
</tr>
<tr>
<td>Zeta</td>
<td>Ζ</td>
<td>ζ</td>
</tr>
<tr>
<td>Eta</td>
<td>Η η</td>
<td>η</td>
</tr>
<tr>
<td>Theta</td>
<td>Θ 0, θ</td>
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</tr>
<tr>
<td>Iota</td>
<td>Ι ι</td>
<td></td>
</tr>
<tr>
<td>Kappa</td>
<td>Κ κ</td>
<td></td>
</tr>
<tr>
<td>Lambda</td>
<td>Λ λ</td>
<td></td>
</tr>
<tr>
<td>Mu</td>
<td>М µ</td>
<td></td>
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<tr>
<td>Nu</td>
<td>N ν</td>
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<tr>
<td>Xi</td>
<td>Ξ ξ</td>
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<tr>
<td>Omicron</td>
<td>Ο ϖ</td>
<td>o</td>
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<tr>
<td>Pi</td>
<td>Π π</td>
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<tr>
<td>Rho</td>
<td>Р ρ</td>
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</tr>
<tr>
<td>Sigma</td>
<td>Σ σ</td>
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<tr>
<td>Tau</td>
<td>Τ τ</td>
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</tr>
<tr>
<td>Upsilon</td>
<td>Υ υ</td>
<td></td>
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<tr>
<td>Phi</td>
<td>Φ φ, ϕ</td>
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<tr>
<td>Chi</td>
<td>Χ χ</td>
<td></td>
</tr>
<tr>
<td>Psi</td>
<td>Ψ ψ</td>
<td></td>
</tr>
<tr>
<td>Omega</td>
<td>Ω ω</td>
<td></td>
</tr>
</tbody>
</table>

Script and Open-Faced Letters

➤ Script (.await) and open-faced (ℝ; also known as blackboard boldface) letters are available but should not be used routinely. For open-faced letters, only uppercase is available.

Spacing

➤ Leave a space before and after functions set in roman type, unless the argument is enclosed in parentheses, brackets, or braces.

\[
\begin{align*}
\log 2 & \quad \exp(-x) \\
-\log x & \quad \cosh(\beta e\phi) \\
4 \sin \theta & \quad 4 \tan(2y) \\
\tan^2 y & \quad \text{erfc}(y)
\end{align*}
\]
Leave a space before and after mathematical operators that function as verbs or conjunctions; that is, they have numbers on both sides or a symbol for a variable on one side and a number on the other.

\[
\begin{align*}
20 \pm 2\% & \quad p < 0.01 \\
3.24 \pm 0.01 & \quad T_b = 176 \, ^\circ C \\
4 \times 5 \, \text{cm} & \quad n = 25 \\
8 \times 10^{-4} & \quad 1 \, \text{in.} = 2.54 \, \text{cm} \\
k \geq 420 \, \text{s}^{-1} &
\end{align*}
\]

**Exception 1** Leave no space around mathematical operators in subscripts and superscripts.

\[
\Delta H^{n-1} \\
E_{k>353} \\
M^{(x+y)+}
\]

**Exception 2** Leave no space around a slash (\(a/b\)), a ratio colon (1:10), or a centered dot (\(P \cdot M\)).

Leave no space between simple variables being multiplied: \(xy\). Do not use a centered dot (\(\cdot\)) or the times sign (\(\times\)) with single-letter scalar variables.

In multiplication involving the two-letter symbols for transport properties, use a space, enclose them in parentheses, or use the times sign. When superscripts or subscripts are present, the symbols can be closed up.

\[
\begin{align*}
Re \, Nu & \\
(Re)(Nu) & \\
Re \times Nu & \\
Re, Nu &
\end{align*}
\]

Use a space for simple multiplication of functions of the type \(f(x)\) (one-dimensional) or \(g(y, z)\) (multidimensional). Close up multipliers to such functions where applicable. You may also use additional enclosing marks instead of spaces.

\[
W = 2f(x) \, g(y, z) \\
W = 2[f(x)] [g(y, z)]
\]

When mathematical symbols are used as adjectives, that is, with one number that is not part of a mathematical operation, do not leave a space between the symbol and the number.

\[
\begin{align*}
-12 \, ^\circ C & \quad \text{a conversion of } >50\% \\
25 \, \text{g} \ (\pm 1\%) & \quad \text{a probability of } <0.01 \\
at \, 400\times \, \text{magnification} & \\
The \text{level can vary from } -15 \text{ to } +25 \, \text{m}.
\end{align*}
\]
Enclosing Marks

➤ Use enclosing marks (parentheses, brackets, and braces, also called fences) in accordance with the rules of mathematics. Enclose parentheses within square brackets, and square brackets within braces: 

➤ Use enclosing marks around arguments when necessary for clarity.

\[
\sin(x + 1) \\
\sin[2\pi(x - y)/n] \\
\log[-V(r)/kT]
\]

➤ Do not use square brackets, parentheses, or braces around the symbol for a quantity to make it represent any other quantity.

INCORRECT

where \( V \) is volume and \((V)\) is volume at equilibrium

CORRECT

where \( V \) is volume and \( V_e \) is volume at equilibrium

Subscripts and Superscripts

➤ Use italic type for subscripts and superscripts that are themselves symbols for physical quantities or numbers. Use roman type for subscripts and superscripts that are abbreviations and not symbols.

\( C_p \) for heat capacity at constant pressure
\( C_B \) for heat capacity of substance B
\( C_g \) where g is gas
\( E_i \) for energy of the \( i \)th level, where \( i \) is a number
\( g_n \) where n is normal
\( \mu_r \) where r is relative
\( E_k \) where k is kinetic
\( \xi_e \) where e is electric

➤ In most cases, staggered subscripts and superscripts are preferred. Exponents should follow subscripts.

\[
\begin{align*}
&x_1^2 & & T_{2m}^{-1} \\
&C_x^{1/2} & & \Delta H_1^\dagger \\
& & & E_{ads}^\circ \\
& & & B_2^{expd}
\end{align*}
\]
➤ Use a slash (/) in all subscript and superscript fractions, with no space on either side.

\[ \frac{t_{1/2}}{x^{1/2}} \quad M^{2/3} \quad f_{a/b} \]

➤ Leave no space around operators in subscripts and superscripts.

\[ M^{(2-n)^+} \quad E_{T+\theta} \]

➤ Leave no space around other expressions in subscripts and superscripts, unless confusion or misreading would result.

\[ Q_{n-Bu(750^\circ C)} \quad \beta_{\text{zero level}} \quad E_{365\text{nm}} \]

➤ The terms \( e^a \) and \( \exp a \) have the same meaning and can be interchanged. When an exponent to the base \( e \) is very long or complicated, replace the \( e \) with \( \exp \) and place the exponent on line and in enclosing marks. Leave no space between \( \exp \) and the opening enclosing mark.

\[
\exp(\int y \, dt) \quad (\text{not } e^{\int y \, dt})
\]

\[
\exp\left\{ \frac{1}{2} kT\left[y(a + b) - Z\right] \right\} \quad (\text{not } e^{\frac{1}{2} kT\left[y(a + b) - Z\right]})
\]

➤ In running text, do not use the radical sign (\( \sqrt{\cdot} \)) with long terms. Use enclosing marks around the term and a superscript \( 1/2, 1/3, 1/4 \) (etc.) for square, cube, fourth root (etc.), respectively.

\[ (x - y^2)^{1/3} \]

\[ [\sinh^2 u + (\cosh u - 1)^2]^{1/2} \]

**Abbreviations and Symbols**

➤ Certain abbreviations are used only in the context of mathematical equations. Define all of these the first time they are used.

- \( \text{lhs} \) left-hand side (of an equation)
- \( \text{rhs} \) right-hand side (of an equation)
- \( \text{ODE} \) ordinary differential equation
- \( \text{rms} \) root mean square
- \( \text{rmse} \) root-mean-square deviation
- \( \text{s.t.} \) subject to
- \( \text{wrt, WRT} \) with respect to

➤ Some standard usages and symbols for mathematical operations and constants need never be defined. They include the following:

- \( e \) natural base (approximately 2.7183)
- \( \exp x, e^x \) exponential of \( x \)
- \( i \) \( \sqrt{-1} \)
- \( \ln x \) natural logarithm of \( x \)
Equations

Mathematical equations can be presented within running text or displayed on lines by themselves. Follow the guidelines for style and usage just described under “Usage and Style for Symbols” (starting on p 211).
Leave a space

- before and after mathematical signs used as operators (=, ≠, ≡, ∼, ≈, ≅, >, <, +, −, ×, ÷, U, ⊂, ⊆, ∈, etc., but not slash (/), ratio colon, or centered dot), except when they appear in superscripts or subscripts
- before trigonometric and other functions set in roman type
- after trigonometric and other functions set in roman type when their arguments are not in enclosing marks
- before and after derivatives: \( \int \int f(x) \, dx \, f(y) \, dy \) or \( \int x \, dx \)
- between built-up (display) fractions as components of products:
  \[
  \frac{a}{b} \frac{c}{d}
  \]
  or write on one line and clarify with enclosing marks and no space:
  \( (a/b)(c/d) \)
- between functions as components of products: \( W = 2f(x) \, g(y, z) \)

Leave no space

- between single-item variables being multiplied
- in any part of a superscript or subscript, unless confusion or misreading would result
- between any character and its own superscript, prime, or subscript
- on either side of a colon used for a ratio
- on either side of a centered dot
- on either side of a slash (/)
- after mathematical operators used as adjectives: \(-10\)
- after functions when the argument is in parentheses: \( \tanh(\lambda/2) \)
- between an opening parenthesis, bracket, or brace and the next character: \((2x)y\)
- between a closing parenthesis, bracket, or brace and the previous character: \(2(xy)\)
- between back-to-back parentheses, brackets, and braces, e.g., \( ](\)\)
- between nested parentheses, brackets, and braces, e.g., \( [(\)\)
- in any part of limits to summations, products, and integrals
- in any part of lower limits to \( \text{min, max, lim, and inf} \)

Use or do not use spaces around ellipses, depending on the treatment of other items in the series.

- no spaces: \( a_n a_{n+1} a_{n+2} \ldots a_{n+36} \)
- spaces: \( a_n + a_{n+1} + a_{n+2} + \ldots + a_{n+36} \)
- space before: \( a, b, \ldots, x \)
Use enclosing marks in accordance with the rules of mathematics. If the slash (/) is used in division and if there is any doubt where the numerator ends or where the denominator starts, use enclosing marks for one or the other or both.

\[(x + y)/(3x - y)\]

\[(a/b)/c, \text{ or } a/(b/c)\] but never \(a/b/c\)

\[\frac{x + y}{2} = z\] would be better as \((x + y)/2 = z\)

\[\frac{x + y}{z} + 2a\] would be better as \([(x + y)/z] + 2a\)

If an equation is very short and will not be referred to again, you may run it into the text.

A fluid is said to be Newtonian when it obeys Newton’s law of viscosity, given by \(\tau = \eta \gamma\), where \(\tau\) is the shear stress, \(\eta\) is the fluid dynamic constant, and \(\gamma\) is the shear rate.

You may use mathematical expressions as part of a sentence when the subject, verb, and object are all part of the mathematical expression.

When \(V = 12\), eq 15 is valid.

\((V\text{ is the subject, }=\text{ is the verb, and }12\text{ is the object.})\)

When an equation is too long to fit on one line, break it after an operator that is not within an enclosing mark (parentheses, brackets, or braces) or break it between sets of enclosing marks. Do not break equations after integral, product, and summation signs; after trigonometric and other functions set in roman type; or before derivatives.

Number displayed equations by using any consistent system of sequencing.

1, 2, 3, …
1a, 1b, 2, …
I, II, III, …
A, B, C, …
A-1, A-2, A-3, …
B.1, B.2, B.3, …
C1, C2, C3, …

Use equation identifiers in the proper sequence according to appearance in text. Do not skip numbers or letters in the sequence.

Place identifiers in parentheses, flush right on the same line as the equation.

\[V = 64\pi kT\gamma^2 \exp(-\kappa h)\]
An ideal gas law analogy is

$$\pi A = nRT$$

If the principal radii are $R_1$ and $R_2$, then

$$\Delta = R_1 - R_2$$

The area per adsorbed molecule can be calculated from

$$a = N_A \Gamma_S$$

The attractive energy can be approximated by

$$V_A = Ar(12H)^{-1}$$

The simplest method is to use a mapping potential of the form

$$\varepsilon_m = (1 - \lambda_m)\varepsilon_A + \lambda_m\varepsilon_B$$

Marshall developed an equation for rapid coagulation:

$$n = 1 + S\pi Drt$$

The capillary pressure $P$ depends significantly on the wetting contact angle according to

$$P = 2\gamma \cos(\theta/r)$$

where $\gamma$ is the surface tension, $\theta$ is the wetting contact angle, and $r$ is the radius of the capillary.

To cite an equation in text, use the abbreviation “eq” if it is not the first word of the sentence. Spell out “equation” when it is the first word of a sentence or when it is not accompanied by a number. The plural of “eq” is “eqs”.

The number of independent points can be calculated from eq 3.

The number of independent points can be calculated from eqs 3 and 4.

Equation 1 is not accurate for distances greater than $10 \mu m$.

Equations 1 and 2 are not accurate for distances greater than $10 \mu m$. 
Some notations differ in text and in display:

<table>
<thead>
<tr>
<th>In display</th>
<th>In text</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sum_{i=1}^{N}$</td>
<td>$\sum_{i=1}^{N}$ or $\sum_{i=1}^{N}$</td>
</tr>
<tr>
<td>$\prod_{k=2}^{n}$</td>
<td>$\prod_{k=2}^{n}$ or $\prod_{k=2}^{n}$</td>
</tr>
<tr>
<td>$\lim_{i=1}$</td>
<td>$\lim_{i=1}$</td>
</tr>
<tr>
<td>$\max_{j=2}$</td>
<td>$\max_{j=2}$</td>
</tr>
<tr>
<td>$\min_{j=k,n}$</td>
<td>$\min_{j=k,n}$</td>
</tr>
</tbody>
</table>

**Ratio and Mixture Notation**

- Use either a colon or a slash (/) to represent a ratio, but not an en dash. Use either a slash or an en dash between components of a mixture, but not a colon.

  - dissolved in 5:1 glycerin/water
  - dissolved in 5:1 glycerin–water
  - the metal/ligand (1:1) reaction mixture
  - the metal–ligand (1:1) reaction mixture
  - the metal–ligand (1/1) reaction mixture
  - the methane/oxygen/argon (1/50/450) matrix
  - the methane/oxygen/argon (1:50:450) matrix

**Set Notation**

The following symbols are used in set notation. Leave a space before and after all operators, but not before and after braces.

- $A = \{a, b\}$ set $A$; $A$ is italic; braces are used
- $A \cup B$ union of sets $A$ and $B$
- $A \cap B$ intersection of sets $A$ and $B$
- $A \in B$ $A$ is a member (element) of $B$
- $A \notin B$ $A$ is not a member (element) of $B$
- $A \subset B$ $A$ is contained in $B$
- $A \not\subset B$ $A$ is not contained in $B$
- $A \supset B$ $A$ contains $B$
- $A \supset B$ $A$ does not contain $B$
- $\forall A$ for all (every) $A$
- $\exists$ there exists
- $\exists$ such that
- $\therefore$ therefore
Geometric Notation
➤ Leave no spaces around geometric notation. Use italic type for planes and axes and roman type for points and lines.

\[ X \perp Y \] \( X \) is perpendicular to \( Y \)

\[ X \parallel Y \] \( X \) is parallel to \( Y \)

\[ \angle AB \] the angle between \( A \) and \( B \)

\[ AB \] length of line from \( A \) to \( B \)

Statistics
Certain statistical symbols are standard.

\[
\begin{align*}
\text{CV} & \quad \text{coefficient of variation} \\
\text{df, DF} & \quad \text{degrees of freedom} \\
\text{f} & \quad \text{frequency} \\
\text{F} & \quad \text{variance ratio} \\
n, N & \quad \text{total number of individuals or random variables} \\
p, P & \quad \text{probability} \\
r & \quad \text{correlation coefficient} \\
R & \quad \text{regression coefficient} \\
\text{RSD} & \quad \text{relative standard deviation} \\
\sigma, SD & \quad \text{standard deviation} \\
\Sigma & \quad \text{summation} \\
s^2 & \quad \text{sample variance} \\
\text{SE} & \quad \text{standard error} \\
\text{SEM} & \quad \text{standard error of the mean} \\
t & \quad \text{Student distribution (the Student } t \text{ test)} \\
\bar{x} & \quad \text{arithmetic mean}
\end{align*}
\]

A common statistical measurement is the Student \( t \) test or Student’s \( t \) test. Student was the pseudonym of W. Gossett, an eminent mathematician.

Units of Measure
➤ Where possible, use metric and SI units (discussed in Appendix 11-1) in all technical documents. The following conventions apply to all units of measure:

- Abbreviate units of measure when they accompany numbers.
- Leave a space between a number and its unit of measure.
- Do not use a period after an abbreviated unit of measure (exception: in. for inch).
• Do not define units of measure.

- 500 mL
- 200 mV
- 3 min
- $4.14 \times 10^{-9}$ m$^2$/V s
- 4 Å
- 2.6 × 10$^4$ J
- 9 V/s
- 3 min interval
- 9 V s$^{-1}$
- 2 µm droplet
- 9 V·s$^{-1}$
- 500 mL flask

**EXCEPTION** Do not leave a space between a number and the percent, angular degree, angular minute, or angular second symbols.

- 50%
- 90°
- 75′
- 18″

➤ Use °C with a space after a number, but no space between the degree symbol and the capital C: 15 °C.

➤ Do not add an “s” to make the plural of any abbreviated units of measure. The abbreviations are used as both singular and plural.

- 50 mg (*not* 50 mgs)
- 3 mol (*not* 3 mols)

➤ Write abbreviated compound units with a centered dot or a space between the units to indicate multiplication and a slash (/) or negative exponent for division. Enclose compound units following a slash in parentheses. Usage should be consistent within a paper.

- watt per meter-kelvin is $W \cdot m^{-1} \cdot K^{-1}$ or $W/(m \cdot K)$ or $W$ m$^{-1}$ K$^{-1}$ or $W$ (m K)$^{-1}$ or $W/$(m K)
- cubic decimeter per mole-second is $dm^3 \cdot mol^{-1} \cdot s^{-1}$ or $dm^3/(mol \cdot s)$ or $dm^3$ mol$^{-1}$ s$^{-1}$ or $dm^3$ (mol s)$^{-1}$ or $dm^3/$(mol s)
- joule per mole-kelvin is $J \cdot mol^{-1} \cdot K^{-1}$ or $J/$(mol·K) or $J$ mol$^{-1}$ K$^{-1}$ or $J$ (mol K)$^{-1}$ or $J/$(mol K)
Spell out units of measure that do not follow a number. Do not capitalize them unless they are at the beginning of a sentence or in a title.

- several milligrams (not several mg)
- a few milliliters (not a few mL)
- degrees Celsius
- reciprocal seconds
- milligrams per kilogram
- volts per square meter

**EXCEPTION 1** Abbreviate units of measure in parentheses after the definitions of variables directly following an equation.

\[ L = \frac{D}{P_0} \]

where \( L \) is the distance between particles (cm), \( D \) is the particle density \( (g/cm^3) \), and \( P_0 \) is the partial pressure of oxygen (kPa).

**EXCEPTION 2** Certain units of measure have no abbreviations: bar, darcy, einstein, erg, faraday, and langmuir. The symbol for the unit torr is Torr. The unit rad is abbreviated rd; the unit radian is abbreviated rad.

**EXCEPTION 3** In column headings of tables and in axis labels of figures, abbreviate units of measure, even without numbers.

Add an “s” to form the plural of spelled-out units: milligrams, poises, kelvins, amperes, watts, newtons, and so on.

**EXCEPTIONS** bar, hertz, lux, stokes, siemens, and torr remain unchanged; darcy becomes darcies; henry becomes henries.

Do not capitalize surnames that are used as units of measure.

- ampere
- angstrom
- coulomb
- curie
- dalton
- darcy
- debye
- einstein
- erg
- faraday
- franklin
- gauss
- gilbert
- gray
- hartree
- henry
- hertz
- joule
- kelvin
- langmuir
- newton
- ohm
- pascal
- poise
- siemens
- sievert
- stokes
- tesla
- watt
- weber

Celsius and Fahrenheit are always capitalized. They are not themselves units; they are the names of temperature scales.

Do not use a slash (/) in spelled-out units of measure. Use the word “per”.

Results are reported in meters per second.

The fluid density is given in kilograms per cubic meter.
Do not mix abbreviations and spelled-out units within units of measure.

- newtons per meter (not N per meter)
- 100 F/m (not 100 farad/m)

**Exception** in more complex situations

- 50 mL of water and 20 mg of NaOH per gram of compound

Use a slash (/), not the word “per”, before the abbreviation for a unit in complex expressions.

- 50 μg of peptide/mL
- 25 mg of drug/kg of body weight

When the first part of a unit of measure is a word that is not itself a unit of measure, use a slash (/) before the final abbreviated unit.

- 10 counts/s
- 12 domains/cm$^3$
- $2 \times 10^3$ ions/min
- 125 conversions/mm$^2$

When the last part of a unit of measure is a word that is not itself a unit of measure, use either a slash (/) or the word “per” before the word that is not a unit.

- 0.8 keV/channel
- 0.8 keV per channel
- 7 μg/boron
- 7 μg per boron

Leave no space between the multiplying prefix and the unit, whether abbreviated or spelled out.

- kilojoule or kJ
- milligram or mg
- microampere or μA

Use only one multiplicative prefix per unit.

- nm (not μm)

In ranges and series, retain only the final unit of measure.

- 10–12 mg
- 5, 10, and 20 kV
- 60–90°
- between 25 and 50 mL
- from 10 to 15 min
➤ Do not use the degree symbol with kelvin: 115 K.

➤ In titles and headings, do not capitalize abbreviated units of measure that are ordinarily lowercase.

   Analysis of 2 mg Samples

   A 50 kDa Protein To Modulate Guanine Nucleotide Binding
The International System of Units (SI)

Before the 1960s, four systems of units were commonly used in the scientific literature: the English system (centuries old, using yard and pound), the metric system (dating from the 18th century, using meter and kilogram as standard units), the CGS system (based on the metric system, using centimeter, gram, and second as base units), and the MKSA or Giorgi system (using meter, kilogram, second, and ampere as base units).

The International System of Units (SI, Système International d’Unités) is the most recent effort to develop a coherent system of units. It is coherent because there is only one unit for each base physical quantity, and units for all other quantities are derived from these base units by simple equations. It has been adopted as a universal system to simplify communication of numerical data and to restrict proliferation of systems. SI units are used by the National Institute of Standards and Technology (NIST). More information on SI can be found at http://www.physics.nist.gov/cuu/index.html.

The SI is constructed from seven base units for independent quantities (ampere, candela, kelvin, kilogram, meter, mole, and second) plus two supplementary units for plane and solid angles (radian and steradian). Most physicochemical measurements can be expressed in terms of these units.

Certain units not part of the SI are so widely used that it is impractical to abandon them (e.g., liter, minute, and hour) or are so well established that the International Committee on Weights and Measures has authorized their continued use (e.g., bar, curie, and angstrom). In addition, quantities that are expressed in terms of the fundamental constants of nature, such as elementary charge, proton mass, Bohr magneton, speed of light, and Planck constant, are also acceptable. However, broad terms such as “atomic units” are not acceptable, although atomic mass unit, u, is acceptable and relevant to chemistry.

Follow all usage conventions given for units of measure. Use the abbreviations for SI units with capital and lowercase letters exactly as they appear in Tables 11A-1 to 11A-6.
### Table 11A-1. SI Units

<table>
<thead>
<tr>
<th>Name</th>
<th>Symbol</th>
<th>Physical Quantity</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Base units</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ampere</td>
<td>A</td>
<td>electric current</td>
</tr>
<tr>
<td>candela</td>
<td>cd</td>
<td>luminous intensity</td>
</tr>
<tr>
<td>kelvin</td>
<td>K</td>
<td>thermodynamic temperature</td>
</tr>
<tr>
<td>kilogram</td>
<td>kg</td>
<td>mass</td>
</tr>
<tr>
<td>meter</td>
<td>m</td>
<td>length</td>
</tr>
<tr>
<td>mole</td>
<td>mol</td>
<td>amount of substance</td>
</tr>
<tr>
<td>second</td>
<td>s</td>
<td>time</td>
</tr>
<tr>
<td><strong>Supplementary units</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>radian</td>
<td>rad</td>
<td>plane angle</td>
</tr>
<tr>
<td>steradian</td>
<td>sr</td>
<td>solid angle</td>
</tr>
</tbody>
</table>

### Table 11A-2. Multiplying Prefixes

<table>
<thead>
<tr>
<th>Factor</th>
<th>Prefix</th>
<th>Symbol</th>
<th>Factor</th>
<th>Prefix</th>
<th>Symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>10⁻²⁴</td>
<td>yocto</td>
<td>y</td>
<td>10¹</td>
<td>deka</td>
<td>da</td>
</tr>
<tr>
<td>10⁻²¹</td>
<td>zepto</td>
<td>z</td>
<td>10²</td>
<td>hecto</td>
<td>h</td>
</tr>
<tr>
<td>10⁻¹⁸</td>
<td>atto</td>
<td>a</td>
<td>10³</td>
<td>kilo</td>
<td>k</td>
</tr>
<tr>
<td>10⁻¹⁵</td>
<td>femto</td>
<td>f</td>
<td>10⁶</td>
<td>mega</td>
<td>M</td>
</tr>
<tr>
<td>10⁻¹²</td>
<td>pico</td>
<td>p</td>
<td>10⁹</td>
<td>giga</td>
<td>G</td>
</tr>
<tr>
<td>10⁻⁹</td>
<td>nano</td>
<td>n</td>
<td>10¹²</td>
<td>tera</td>
<td>T</td>
</tr>
<tr>
<td>10⁻⁶</td>
<td>micro</td>
<td>µ</td>
<td>10¹⁵</td>
<td>peta</td>
<td>P</td>
</tr>
<tr>
<td>10⁻³</td>
<td>milli</td>
<td>m</td>
<td>10¹⁸</td>
<td>exa</td>
<td>E</td>
</tr>
<tr>
<td>10⁻²</td>
<td>centi</td>
<td>c</td>
<td>10²¹</td>
<td>zetta</td>
<td>Z</td>
</tr>
<tr>
<td>10⁻¹</td>
<td>deci</td>
<td>d</td>
<td>10²⁴</td>
<td>yotta</td>
<td>Y</td>
</tr>
</tbody>
</table>

Note: Any of these prefixes may be combined with any of the symbols permitted within the SI. Thus, kPa and GPa will both be common combinations in measurements of pressure, as will mL and cm for measurements of volume and length, respectively. As a general rule, however, the prefix chosen should be 10 raised to that multiple of 3 that will bring the numerical value of the quantity to a positive value less than 1000.

### Table 11A-3. SI-Derived Units

<table>
<thead>
<tr>
<th>Name</th>
<th>Symbol</th>
<th>Quantity</th>
</tr>
</thead>
<tbody>
<tr>
<td>becquerel</td>
<td>Bq</td>
<td>activity (of a radionuclide)</td>
</tr>
<tr>
<td>coulomb</td>
<td>C</td>
<td>quantity of electricity, electric charge</td>
</tr>
<tr>
<td>farad</td>
<td>F</td>
<td>capacitance</td>
</tr>
<tr>
<td>gray</td>
<td>Gy</td>
<td>absorbed dose, kerma, specific energy imparted</td>
</tr>
<tr>
<td>henry</td>
<td>H</td>
<td>inductance</td>
</tr>
<tr>
<td>hertz</td>
<td>Hz</td>
<td>frequency</td>
</tr>
<tr>
<td>joule</td>
<td>J</td>
<td>energy, work, quantity of heat</td>
</tr>
<tr>
<td>lumen</td>
<td>lm</td>
<td>luminous flux</td>
</tr>
<tr>
<td>lux</td>
<td>lx</td>
<td>illuminance</td>
</tr>
<tr>
<td>newton</td>
<td>N</td>
<td>force</td>
</tr>
<tr>
<td>ohm</td>
<td>Ω</td>
<td>electric resistance</td>
</tr>
<tr>
<td>pascal</td>
<td>Pa</td>
<td>pressure, stress</td>
</tr>
<tr>
<td>siemens</td>
<td>S</td>
<td>conductance</td>
</tr>
<tr>
<td>sievert</td>
<td>Sv</td>
<td>dose equivalent</td>
</tr>
<tr>
<td>tesla</td>
<td>T</td>
<td>magnetic flux density</td>
</tr>
<tr>
<td>volt</td>
<td>V</td>
<td>electric potential, potential difference, electromotive force</td>
</tr>
<tr>
<td>watt</td>
<td>W</td>
<td>power, radiant flux</td>
</tr>
<tr>
<td>weber</td>
<td>Wb</td>
<td>magnetic flux</td>
</tr>
</tbody>
</table>
### Table 11A-4. SI-Derived Compound Units

<table>
<thead>
<tr>
<th>Name</th>
<th>Symbol</th>
<th>Quantity</th>
<th>In Terms Of Other Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>ampere per meter</td>
<td>A/m</td>
<td>magnetic field strength</td>
<td>—</td>
</tr>
<tr>
<td>ampere per square meter</td>
<td>A/m²</td>
<td>current density</td>
<td>—</td>
</tr>
<tr>
<td>candela per square meter</td>
<td>cd/m²</td>
<td>luminance</td>
<td>—</td>
</tr>
<tr>
<td>coulomb per cubic meter</td>
<td>C/m³</td>
<td>electric charge density</td>
<td>m⁻³·s·A⁻¹</td>
</tr>
<tr>
<td>coulomb per kilogram</td>
<td>C/kg</td>
<td>exposure (X-rays and γ rays)</td>
<td>—</td>
</tr>
<tr>
<td>coulomb per square meter</td>
<td>C/m²</td>
<td>electric flux density</td>
<td>m⁻²·s·A⁻¹</td>
</tr>
<tr>
<td>cubic meter</td>
<td>m³</td>
<td>volume</td>
<td>—</td>
</tr>
<tr>
<td>cubic meter per kilogram</td>
<td>m³/kg</td>
<td>specific volume</td>
<td>—</td>
</tr>
<tr>
<td>farad per meter</td>
<td>F/m</td>
<td>permittivity</td>
<td>m⁻³·kg⁻¹·s⁻⁴·A⁻²</td>
</tr>
<tr>
<td>henry per meter</td>
<td>H/m</td>
<td>permeability</td>
<td>m·kg·s⁻²·A⁻²</td>
</tr>
<tr>
<td>joule per cubic meter</td>
<td>J/m³</td>
<td>energy density</td>
<td>m⁻¹·kg·s⁻²</td>
</tr>
<tr>
<td>joule per kelvin</td>
<td>J/K</td>
<td>heat capacity, entropy</td>
<td>m²·kg·s⁻²·K⁻¹</td>
</tr>
<tr>
<td>joule per kilogram</td>
<td>J/kg</td>
<td>specific energy</td>
<td>m²·s⁻²</td>
</tr>
<tr>
<td>joule per kilogram kelvin</td>
<td>J/(kg K)</td>
<td>specific heat capacity, specific entropy</td>
<td>m²·s⁻²·K⁻¹</td>
</tr>
<tr>
<td>joule per mole</td>
<td>J/mol</td>
<td>molar energy</td>
<td>m²·kg·s⁻²·mol⁻¹</td>
</tr>
<tr>
<td>joule per mole kelvin</td>
<td>J/(mol K)</td>
<td>molar entropy, molar heat capacity</td>
<td>m²·kg·s⁻²·K⁻¹·mol⁻¹</td>
</tr>
<tr>
<td>kilogram per cubic meter</td>
<td>kg/m³</td>
<td>density, mass density</td>
<td>—</td>
</tr>
<tr>
<td>meter per second</td>
<td>m/s</td>
<td>speed, velocity</td>
<td>—</td>
</tr>
<tr>
<td>meter per second squared</td>
<td>m/s²</td>
<td>acceleration</td>
<td>—</td>
</tr>
<tr>
<td>mole per cubic meter</td>
<td>mol/m³</td>
<td>concentration (amount of substance per volume)</td>
<td>—</td>
</tr>
<tr>
<td>newton-meter</td>
<td>N·m</td>
<td>moment of force</td>
<td>m²·kg·s⁻²</td>
</tr>
<tr>
<td>newton per meter</td>
<td>N/m</td>
<td>surface tension</td>
<td>kg·s⁻²</td>
</tr>
<tr>
<td>pascal second</td>
<td>Pa·s</td>
<td>dynamic viscosity</td>
<td>m⁻¹·kg·s⁻¹</td>
</tr>
<tr>
<td>radian per second</td>
<td>rad/s</td>
<td>angular velocity</td>
<td>—</td>
</tr>
<tr>
<td>radian per second squared</td>
<td>rad/s²</td>
<td>angular acceleration</td>
<td>—</td>
</tr>
<tr>
<td>reciprocal meter</td>
<td>m⁻¹</td>
<td>wavenumber</td>
<td>—</td>
</tr>
<tr>
<td>reciprocal second</td>
<td>s⁻¹</td>
<td>frequency</td>
<td>—</td>
</tr>
<tr>
<td>square meter</td>
<td>m²</td>
<td>area</td>
<td>—</td>
</tr>
<tr>
<td>square meter per second</td>
<td>m²/s</td>
<td>kinematic viscosity</td>
<td>—</td>
</tr>
<tr>
<td>volt per meter</td>
<td>V/m</td>
<td>electric field strength</td>
<td>m·kg·s⁻³·A⁻¹</td>
</tr>
<tr>
<td>watt per meter kelvin</td>
<td>W/(m K)</td>
<td>thermal conductivity</td>
<td>m·kg·s⁻³·K⁻¹</td>
</tr>
<tr>
<td>watt per square meter</td>
<td>W/m²</td>
<td>heat flux density, irradiance</td>
<td>kg·s⁻³</td>
</tr>
<tr>
<td>watt per square meter steradian</td>
<td>W/(m² sr)</td>
<td>radiance</td>
<td>—</td>
</tr>
<tr>
<td>watt per steradian</td>
<td>W/sr</td>
<td>radiant intensity</td>
<td>—</td>
</tr>
</tbody>
</table>

*Liter (L) is a special name for cubic decimeter. The symbol M is not an SI unit, but expressions such as 0.1 M, meaning a solution with concentration of 0.1 mol/L, are acceptable.*
## Table 11A-5. Other Units

<table>
<thead>
<tr>
<th>Name</th>
<th>Symbol</th>
<th>Quantity</th>
<th>Value in SI Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>angstrom</td>
<td>Å</td>
<td>distance</td>
<td>1 Å = 10⁻¹⁰ m = 0.1 nm</td>
</tr>
<tr>
<td>bar</td>
<td>bar</td>
<td>pressure</td>
<td>1 bar = 10⁵ Pa = 100 kPa = 0.1 MPa</td>
</tr>
<tr>
<td>barn</td>
<td>b, bₚ</td>
<td>area, cross section</td>
<td>1 b = 10⁻²⁸ m² = 100 fm²</td>
</tr>
<tr>
<td>bohr</td>
<td>bₒ</td>
<td>length</td>
<td>1 b ≈ 5.291 77 × 10⁻¹¹ m</td>
</tr>
<tr>
<td>curie</td>
<td>Ci</td>
<td>activity</td>
<td>1 Ci = 3.7 × 10¹⁰ Bq</td>
</tr>
<tr>
<td>dalton</td>
<td>Da</td>
<td>atomic mass</td>
<td>1 Da = 1.660 540 × 10⁻²⁷ kg</td>
</tr>
<tr>
<td>darcy</td>
<td>darcy</td>
<td>permeability</td>
<td>—</td>
</tr>
<tr>
<td>day</td>
<td>day</td>
<td>time</td>
<td>1 day = 24 h = 86 400 s</td>
</tr>
<tr>
<td>debye</td>
<td>D</td>
<td>electric dipole moment</td>
<td>—</td>
</tr>
<tr>
<td>degree</td>
<td>°</td>
<td>plane angle</td>
<td>1° = (π/180) rad</td>
</tr>
<tr>
<td>degree Celsius</td>
<td>°C</td>
<td>temperature</td>
<td>—</td>
</tr>
<tr>
<td>dyn</td>
<td>dyn</td>
<td>force</td>
<td>—</td>
</tr>
<tr>
<td>einstein</td>
<td>ein</td>
<td>light energy</td>
<td>—</td>
</tr>
<tr>
<td>electronvolt</td>
<td>eV</td>
<td>—</td>
<td>1 eV = 1.602 19 × 10⁻¹⁹ J</td>
</tr>
<tr>
<td>erg</td>
<td>erg</td>
<td>energy or work</td>
<td>—</td>
</tr>
<tr>
<td>faraday</td>
<td>faraday</td>
<td>electric charge</td>
<td>1 faraday = 96 485.31 C</td>
</tr>
<tr>
<td>fermi</td>
<td>f</td>
<td>length</td>
<td>1 f = 10⁻¹⁵ m</td>
</tr>
<tr>
<td>franklin</td>
<td>Fr</td>
<td>electric charge</td>
<td>1 Fr = 3.335 64 × 10⁻¹⁰ C</td>
</tr>
<tr>
<td>galileo</td>
<td>Gal</td>
<td>acceleration</td>
<td>1 Gal = 10⁻² m s⁻²</td>
</tr>
<tr>
<td>gauss</td>
<td>G</td>
<td>magnetic induction</td>
<td>1 G = 10⁻⁴ Wb/m²</td>
</tr>
<tr>
<td>gilbert</td>
<td>Gi</td>
<td>magnetomotive force</td>
<td>—</td>
</tr>
<tr>
<td>hartree</td>
<td>hartree, Eₜ</td>
<td>energy</td>
<td>1 hartree = 4.359 75 × 10⁻¹⁸ J</td>
</tr>
<tr>
<td>hectare</td>
<td>ha</td>
<td>area</td>
<td>1 ha = 1 hm² = 10⁴ m²</td>
</tr>
<tr>
<td>hour</td>
<td>h</td>
<td>time</td>
<td>1 h = 60 min = 3600 s</td>
</tr>
<tr>
<td>liter</td>
<td>L</td>
<td>volume</td>
<td>1 L = 1 dm³ = 10⁻³ m³</td>
</tr>
<tr>
<td>metric ton</td>
<td>t</td>
<td>mass</td>
<td>1 t = 10³ kg</td>
</tr>
<tr>
<td>minute</td>
<td>min</td>
<td>time</td>
<td>1 min = 60 s</td>
</tr>
<tr>
<td>minute</td>
<td>°</td>
<td>plane angle</td>
<td>1° = (1/60)° = (π/10 800) rad</td>
</tr>
<tr>
<td>parsec</td>
<td>pc</td>
<td>length</td>
<td>1 pc ≈ 3.085 68 × 10⁻¹⁶ m</td>
</tr>
<tr>
<td>poise</td>
<td>P</td>
<td>dynamic viscosity</td>
<td>—</td>
</tr>
<tr>
<td>rad</td>
<td>rad, rd</td>
<td>absorbed dose</td>
<td>1 rad = 0.01 Gy = 1 cGy = 100 erg·g⁻¹</td>
</tr>
<tr>
<td>roentgen</td>
<td>R</td>
<td>exposure</td>
<td>1 R = 2.58 × 10⁻⁴ C·kg⁻¹</td>
</tr>
<tr>
<td>roentgen equivalent</td>
<td>rem</td>
<td>weighted absorbed dose</td>
<td>1 rem = 0.01 Sv</td>
</tr>
<tr>
<td>man¹</td>
<td></td>
<td></td>
<td>—</td>
</tr>
<tr>
<td>second</td>
<td>°</td>
<td>plane angle</td>
<td>1°° = (1/60)°° = (π/648 000) rad</td>
</tr>
<tr>
<td>stokes</td>
<td>St</td>
<td>kinematic viscosity</td>
<td>—</td>
</tr>
<tr>
<td>svedberg</td>
<td>Sv</td>
<td>time</td>
<td>1 Sv = 10⁻¹³ s</td>
</tr>
<tr>
<td>unified atomic mass</td>
<td>u</td>
<td>—</td>
<td>1 u = 1.660 540 × 10⁻²⁷ kg</td>
</tr>
</tbody>
</table>

---

*a1 Ci = 2.2 × 10¹² disintegrations per minute.  
b1 darcy is the permeation achieved by the passage of 1 mL of fluid of 1 cP viscosity flowing in 1 s under a pressure of 1 atm (101 kPa) through a porous medium that has a cross-sectional area of 1 cm² and a length of 1 cm.  
c1 D = 10⁻¹⁸ Fr cm.  
d1 Temperature intervals in kelvins and degrees Celsius are identical; however, temperature in kelvins equals temperature in degrees Celsius plus 273.15.  
e1 1 einstein equals Avogadro’s number times the energy of one photon of light at the frequency in question.  
f1 The electronvolt is the kinetic energy acquired by an electron in passing through a potential difference of 1 V in vacuum.  
g1 1 erg is the work done by a 1 dyn force when the point at which the force is applied is displaced by 1 cm in the direction of the force.  
h1 1 Gi is the magnetomotive force of a closed loop of one turn in which there is a current of (1/4π) × 10 A.  
i1 P is the dynamic viscosity of a fluid in which there is a tangential force of 1 dyn/cm² resisting the flow of two parallel fluid layers past each other when their differential velocity is 1 cm/s per centimeter of separation.  
j1 When there is a possibility of confusion with the symbol for radian, rd may be used as the symbol for rad.  
k1 rem has the same biological effect as 1 rad of X-rays.  
m1 St is the kinematic viscosity of a fluid with a dynamic viscosity of 1 P and a density of 1 g/cm³.  
n1 The unified atomic mass unit is equal to 1/12 of the mass of an atom of the nuclide ¹²C.
Table 11A-6. Non-SI Units That Are Discouraged

<table>
<thead>
<tr>
<th>Discouraged Unit</th>
<th>Value in SI Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>calorie (thermochemical)</td>
<td>4.184 J</td>
</tr>
<tr>
<td>conventional millimeter of mercury</td>
<td>133.322 Pa</td>
</tr>
<tr>
<td>grad</td>
<td>2π/400 rad</td>
</tr>
<tr>
<td>kilogram-force</td>
<td>9.806 65 N</td>
</tr>
<tr>
<td>metric carat</td>
<td>0.2 g</td>
</tr>
<tr>
<td>metric horsepower</td>
<td>735.499 W</td>
</tr>
<tr>
<td>mho</td>
<td>1 S</td>
</tr>
<tr>
<td>micron</td>
<td>1 µm</td>
</tr>
<tr>
<td>standard atmosphere</td>
<td>101.325 kPa</td>
</tr>
<tr>
<td>technical atmosphere</td>
<td>98.066 5 kPa</td>
</tr>
<tr>
<td>torr</td>
<td>133.322 Pa</td>
</tr>
</tbody>
</table>
The use of proper chemical nomenclature is essential for effective scientific communication. More than one million new substances are reported each year, each of which must be identified clearly, unambiguously, and completely in the primary literature. Chemical compounds are named according to the rules established by the International Union of Pure and Applied Chemistry (IUPAC), the International Union of Biochemistry and Molecular Biology (IUBMB) [formerly the International Union of Biochemistry (IUB)], the Chemical Abstracts Service (CAS), the Committee on Nomenclature, Terminology, and Symbols of the American Chemical Society, and other authorities as appropriate. For more information on naming chemical compounds, refer to the bibliography in Chapter 18. This chapter gives the editorial conventions and style points for chemical compound names.

Components of Chemical Names

The names of chemical compounds may consist of one or more words, and they may include locants, descriptors, and syllabic portions. Locants and descriptors can be numerals, element symbols, small capital letters, Greek letters, Latin letters, italic words and letters, and combinations of these. Treat the word or syllabic portions of chemical names just like other common nouns: use roman type, keep them lowercase in text, capitalize them at the beginnings of sentences and in titles, and hyphenate them only when they do not fit completely on one line.
Locants and Descriptors

Numerals used as locants can occur at the beginning of or within a chemical name. They are set off with hyphens. (See Box 12-1.)

- 6-aminobenzothiazole
- di-2-propenylcyanamide
- 4a,8a-dihydronaphthalene
- 5,7-dihydroxy-3-(4-hydroxyphenyl)-4H-1-benzopyran-4-one
- 6-hydroxy-2-naphthalenesulfonic acid
- 3′-methylphthalanilic acid

Use italic type for chemical element symbols that denote attachment to an atom or a site of ligation.

- $B,B'$-di-3-pinanyldiborane
- bis[(ethylthio)acetato-O,S]platinum
- glycinato-$N$
- $N$-acetyl group
- $N$-ethylaniline
- $N,N'$-bis(3-aminopropyl)-1,4-butanediamine
- $O,O,S$-triethyl phosphorodithioate
- $P$-phenylphosphinimidic acid
- $S$-methyl benzenethiosulfonate

When element symbols are used with a type of reaction as a noun or adjective, use roman type for the symbol and hyphenate it to the word that follows it.

- N-acetylated
- N-acetylation
- N-oxidation
- N-oxidized
- O-substituted
- O-substitution
- S-methylated
- S-methylation
Use italic type for the capital H that denotes indicated or added hydrogen.

- 1H-1,3-diazepine
- 3H-fluorene
- 2H-indene

Use Greek letters, not the spelled-out forms, in chemical names to denote position or stereochemistry. Use a hyphen to separate them from the chemical name.

- α-amino acid (not alpha amino acid)
- β-naphthol (not beta naphthol)
- 5α,10β,15α,20α-tetraphenylporphyrin

Use the Greek letters eta (η) to indicate hapticity and kappa (κ) to designate the ligating atom in complicated formulas.

- bis(η6-benzene)-chromium
- bis(η-cyclopentadienyl) iron
- [2-(diphenylphosphino-κP)phenyl-κC1]hydrido(triphenylphosphine-κP)-nickel(II)
- N,N'-bis(2-amino-κN-ethyl)ethane-1,2-diamine-κN]chloroplatinum(II)

Use italic type for positional, stereochemical, configurational, and descriptive structural prefixes when they appear with the chemical name or formula. Use a hyphen to separate them from the chemical name. Accepted prefixes include the following:

- abeo
- ac
- altro
- amphi
- anti
- antiprismo
- ar
- arachno
- as
- asym
- c
- catena
- cis
- cisoid
- closo
- cyclo
- d

- dodecahedro
- E
- endo
- erythro
- exo
- facgem
- hexahedro
- hexaprismo
- hypho
- icosahedro
- klado
- l
- m
- M
- mer
- meso
- n

- nido
- o
- octahedro
- P
- pentaprismo
- R
- R*
- rel
- retro
- ribo
- s
- S
- S*
- sec
- sn
- sym
- syn
- t
- tert
- tetraedro
- threo
- trans
- transoid
- triangulo
- triprismo
- uns
- vic
- xylo
- Z

Do not capitalize prefixes that are shown here as lowercase, even at the beginning of a sentence or in a title (see Tables 12-1 and 12-2), and never use lower-
case for those that are written in capital letters. Enclose the prefixes \( E, R, R^*, S, S^*, \) and \( Z \) in parentheses.

- anti-bicyclo[3.2.1]octan-8-amine
- ar-chlorotoluene
- as-trichlorobenzene
- catena-triphosphoric acid
- cis-diamminedichloroplatinum
- cyclo-hexasulfur, \( c-S_6 \)
- \((E,E)-2,4\)-hexadienoic acid
- \((E,Z)-1,3\)-di-1-propenylnaphthalene
- exo-chloro-p-menthane
- \(m\)-ethylpropylbenzene
- \(meso\)-tartaric acid

➤ Use small capital letters \( \text{d} \) and \( \text{l} \) to indicate absolute configuration with amino acids and carbohydrates.

- 2-(difluoromethyl)-\( \text{dI} \)-ornithine
- \( \text{l}\)-galactosamine
- 2-\( O\)-\(\beta\)-d-glucopyranosyl-\(\alpha\)-d-glucose

➤ Use plus and minus signs enclosed in parentheses as stereochemical descriptors.

- \((\pm)-2\)-allylcyclohexanone
- \((+)-\)dihydrocinchonine
- \((-)-3\)-(3,4-dihydroxyphenyl)-\(\text{l}\)-alanine

➤ When the structural prefixes cyclo, iso, neo, and spiro are integral parts of chemical names, close them up to the rest of the name (without hyphens) and do not italicize them.

- cyclohexane
- isopropyl alcohol
- neopentane

However, italicize and hyphenate cyclo as a nonintegral structural descriptor.

- cyclo-octasulfur
- cyclo-triphosphoric acid

➤ Use numerals separated by periods within square brackets in names of bridged and spiro alicyclic compounds.

- bicyclo[3.2.0]heptane
- bicyclo[4.4.0]decane
- 1-methylspiro[3.5]non-5-ene
- spiro[4.5]decane
### Table 12-1. Examples of Multiword Chemical Names

<table>
<thead>
<tr>
<th>In Text</th>
<th>At Beginning of Sentence</th>
<th>In Titles and Headings</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Acids</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>benzoic acid</td>
<td>Benzoic acid</td>
<td>Benzoic Acid</td>
</tr>
<tr>
<td>ethanethioic S-acid</td>
<td>Ethanethioic S-acid</td>
<td>Ethanethioic S-Acid</td>
</tr>
<tr>
<td>hydrochloric acid</td>
<td>Hydrochloric acid</td>
<td>Hydrochloric Acid</td>
</tr>
<tr>
<td><strong>Alcohols</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ethyl alcohol</td>
<td>Ethyl alcohol</td>
<td>Ethyl Alcohol</td>
</tr>
<tr>
<td>ethylene glycol</td>
<td>Ethylene glycol</td>
<td>Ethylene Glycol</td>
</tr>
<tr>
<td><strong>Ketones</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>di-2-naphthyl ketone</td>
<td>Di-2-naphthyl ketone</td>
<td>Di-2-naphthyl Ketone</td>
</tr>
<tr>
<td>methyl phenyl ketone</td>
<td>Methyl phenyl ketone</td>
<td>Methyl Phenyl Ketone</td>
</tr>
<tr>
<td><strong>Ethers</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>di-sec-butyl ether</td>
<td>Di-sec-butyl ether</td>
<td>Di-sec-butyl Ether</td>
</tr>
<tr>
<td>methyl propyl ether</td>
<td>Methyl propyl ether</td>
<td>Methyl Propyl Ether</td>
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<tr>
<td><strong>Anhydrides</strong></td>
<td></td>
<td></td>
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<tr>
<td>acetic anhydride</td>
<td>Acetic anhydride</td>
<td>Acetic Anhydride</td>
</tr>
<tr>
<td>phthalic anhydride</td>
<td>Phthalic anhydride</td>
<td>Phthalic Anhydride</td>
</tr>
<tr>
<td><strong>Esters</strong></td>
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<td>methyl acetate</td>
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<td>phenyl thiocyanate</td>
<td>Phenyl thiocyanate</td>
<td>Phenyl Thiocyanate</td>
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<td>propyl benzoate</td>
<td>Propyl benzoate</td>
<td>Propyl Benzoate</td>
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<tr>
<td><strong>Polymer Names</strong></td>
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<td>1,2-polybutadiene</td>
<td>1,2-Polybutadiene</td>
<td>1,2-Polybutadiene</td>
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<tr>
<td>poly(butyl methacrylate)</td>
<td>Poly(butyl methacrylate)</td>
<td>Poly(butyl methacrylate)</td>
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<td>poly(ethylene glycol)</td>
<td>Poly(ethylene glycol)</td>
<td>Poly(ethylene glycol)</td>
</tr>
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<td>poly((N,N)-dimethylacrylamide)</td>
<td>Poly((N,N)-dimethylacrylamide)</td>
<td>Poly((N,N)-dimethylacrylamide)</td>
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<tr>
<td><strong>Other Organic Compounds</strong></td>
<td></td>
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<tr>
<td>aniline hydrochloride</td>
<td>Aniline hydrochloride</td>
<td>Aniline Hydrochloride</td>
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<tr>
<td>benzyl hydroperoxide</td>
<td>Benzyl hydroperoxide</td>
<td>Benzyl Hydperoxide</td>
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<tr>
<td>butyl chloride</td>
<td>Butyl chloride</td>
<td>Butyl Chloride</td>
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<tr>
<td>dicyclohexyl peroxide</td>
<td>Dicyclohexyl peroxide</td>
<td>Dicyclohexyl Peroxide</td>
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<td>diethyl sulfide</td>
<td>Diethyl sulfide</td>
<td>Diethyl Sulfide</td>
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<tr>
<td>methyl iodide</td>
<td>Methyl iodide</td>
<td>Methyl Iodide</td>
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<td>2-naphthyl bromide</td>
<td>2-Naphthyl bromide</td>
<td>2-Naphthyl Bromide</td>
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<td>sodium S-phenyl thiosulfite</td>
<td>Sodium S-phenyl thiosulfite</td>
<td>Sodium S-Phenyl Thiosulfite</td>
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<td>tert-butyl fluoride</td>
<td>tert-Butyl fluoride</td>
<td>tert-Butyl Fluoride</td>
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<td><strong>Inorganic and Coordination Compounds</strong></td>
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<tr>
<td>ammonium hydroxide</td>
<td>Ammonium hydroxide</td>
<td>Ammonium Hydroxide</td>
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<td>bis(diethyl phosphato)zinc</td>
<td>Bis(diethyl phosphato)zinc</td>
<td>Bis(diethyl phosphato)zinc</td>
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<td>calcium sulfate</td>
<td>Calcium sulfate</td>
<td>Calcium Sulfate</td>
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<td>(dimethyl sulfoxide)-cadmium sulfate</td>
<td>(Dimethyl sulfoxide)-cadmium sulfate</td>
<td>(Dimethyl sulfoxide)-cadmium sulfate</td>
</tr>
<tr>
<td>magnesium oxide</td>
<td>Magnesium oxide</td>
<td>Magnesium Oxide</td>
</tr>
<tr>
<td>sodium cyanide</td>
<td>Sodium cyanide</td>
<td>Sodium Cyanide</td>
</tr>
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<td>sulfur dioxide</td>
<td>Sulfur dioxide</td>
<td>Sulfur Dioxide</td>
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<td>In Text</td>
<td>At Beginning of Sentence</td>
<td>In Titles and Headings</td>
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<tr>
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<td>--------------------------</td>
<td>------------------------</td>
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<tr>
<td><strong>Numerical Locants</strong></td>
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<tr>
<td>adenosine 5′-triphosphate</td>
<td>Adenosine 5′-triphosphate</td>
<td>Adenosine 5′-Triphosphate</td>
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<tr>
<td>1,3-bis(bromomethyl)-benzene</td>
<td>1,3-Bis(bromomethyl)-benzene</td>
<td>1,3-Bis(bromomethyl)-benzene</td>
</tr>
<tr>
<td>2-benzoylbenzoic acid</td>
<td>2-Benzoylbenzoic acid</td>
<td>2-Benzoylbenzoic Acid</td>
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<tr>
<td>1-bromo-3-chloropropane</td>
<td>1-Bromo-3-chloropropane</td>
<td>1-Bromo-3-chloropropane</td>
</tr>
<tr>
<td>2-(2-chloroethyl)pentanoic acid</td>
<td>2-(2-Chloroethyl)pentanoic acid</td>
<td>2-(2-Chloroethyl)pentanoic Acid</td>
</tr>
<tr>
<td>7-(4-chlorophenyl)-1-naphthol</td>
<td>7-(4-Chlorophenyl)-1-naphthol</td>
<td>7-(4-Chlorophenyl)-1-naphthol</td>
</tr>
<tr>
<td>1,2-dicyanobutane</td>
<td>1,2-Dicyanobutane</td>
<td>1,2-Dicyanobutane</td>
</tr>
<tr>
<td>4a,8a-dihydronaphthalene</td>
<td>4a,8a-Dihydronaphthalene</td>
<td>4a,8a-Dihydronaphthalene</td>
</tr>
<tr>
<td><strong>Element Symbol Locants</strong></td>
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<tr>
<td>(2,3-butanedione dioximato-O,O′)copper</td>
<td>(2,3-Butanedione dioximato-O,O′)copper</td>
<td>(2,3-Butanedione dioximato-O,O′)copper</td>
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<tr>
<td>N-ethylaniline</td>
<td>N-Ethylaniline</td>
<td>N-Ethylaniline</td>
</tr>
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<td>N,N′-dihydroxybenzamide</td>
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<td>N,N′-Dihydroxybenzamide</td>
</tr>
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<td>N,N′-dimethylurea</td>
<td>N,N′-Dimethylurea</td>
<td>N,N′-Dimethylurea</td>
</tr>
<tr>
<td>3H-fluorene</td>
<td>3H-Fluorene</td>
<td>3H-Fluorene</td>
</tr>
<tr>
<td>O,S,S-triethyl phosphorodithioate</td>
<td>O,S,S-Triethyl phosphorodithioate</td>
<td>O,S,S-Triethyl Phosphorodithioate</td>
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<tr>
<td>S-methyl benzenethiosulfonate</td>
<td>S-Methyl benzenethiosulfonate</td>
<td>S-Methyl Benzenethiosulfonate</td>
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<td><strong>Greek Letter Locants and Descriptors</strong></td>
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<tr>
<td>α-hydroxy-β-aminobutyric acid</td>
<td>α-Hydroxy-β-aminobutyric acid</td>
<td>α-Hydroxy-β-aminobutyric Acid</td>
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<td>17α-hydroxy-5β-pregnane</td>
<td>17α-Hydroxy-5β-pregnane</td>
<td>17α-Hydroxy-5β-pregnane</td>
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<td>1α-Hydroxycholecalciferol</td>
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<td>α-methylbenzeneacetic acid</td>
<td>α-Methylbenzeneacetic acid</td>
<td>α-Methylbenzeneacetic Acid</td>
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<tr>
<td>α1-sitosterol</td>
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<td>α1-Sitosterol</td>
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<td>β-chloro-1-naphthalenebutanol</td>
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<td>β4-Dichlorocyclohexane-propionic acid</td>
<td>β4-Dichlorocyclohexane-propionic Acid</td>
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<td>β-endorphin</td>
<td>β-Endorphin</td>
<td>β-Endorphin</td>
</tr>
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<td>ω,ω′-dibromopolybutadiene</td>
<td>ω,ω′-Dibromopolybutadiene</td>
<td>ω,ω′-Dibromopolybutadiene</td>
</tr>
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<td>tris(β-chloroethy)lamine</td>
<td>Tris(β-chloroethy)lamine</td>
<td>Tris(β-chloroethy)lamine</td>
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<td><strong>Small Capital Letter Descriptors</strong></td>
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<td>β-α-arabinose</td>
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<td>d-1,2,4-Butanetriol</td>
<td>d-1,2,4-Butanetriol</td>
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<td>d-serine</td>
<td>d-Serine</td>
<td>d-Serine</td>
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<td>dl-alanine</td>
<td>dl-Alanine</td>
<td>dl-Alanine</td>
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<tr>
<td>D-s-threonine</td>
<td>D-s-Threonine</td>
<td>D-s-Threonine</td>
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<tr>
<td>L-methionine</td>
<td>L-Methionine</td>
<td>L-Methionine</td>
</tr>
<tr>
<td><strong>Positional and Structural Descriptors</strong></td>
<td></td>
<td></td>
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<tr>
<td>7-bromo-p-cymene</td>
<td>7-Bromo-p-cymene</td>
<td>7-Bromo-p-cymene</td>
</tr>
<tr>
<td>4-chloro-m-cresol</td>
<td>4-Chloro-m-cresol</td>
<td>4-Chloro-m-cresol</td>
</tr>
<tr>
<td>m-hydroxybenzyl alcohol</td>
<td>m-Hydroxybenzyl alcohol</td>
<td>m-Hydroxybenzyl Alcohol</td>
</tr>
<tr>
<td>n-butyl iodide</td>
<td>n-Butyl iodide</td>
<td>n-Butyl Iodide</td>
</tr>
</tbody>
</table>

Continued on next page
<table>
<thead>
<tr>
<th>Positional and Structural Descriptors — Continued</th>
</tr>
</thead>
<tbody>
<tr>
<td>In Text At Beginning of Sentence In Titles and Headings</td>
</tr>
<tr>
<td>2-(o-chlorophenyl)-1-naphthol</td>
</tr>
<tr>
<td>o-dibromobenzene</td>
</tr>
<tr>
<td>p-benzenedicarboxylic acid</td>
</tr>
<tr>
<td>p-tert-butylphenol</td>
</tr>
<tr>
<td>s-triazine</td>
</tr>
<tr>
<td>sec-butyl alcohol</td>
</tr>
<tr>
<td>sym-dibromoethane</td>
</tr>
<tr>
<td>tert-pentyl isovalerate</td>
</tr>
<tr>
<td>1-(trans-1-propenyl)-3-(cis-1-propenyl)naphthalene</td>
</tr>
<tr>
<td>Stereocchemical Descriptors</td>
</tr>
<tr>
<td>In Text At Beginning of Sentence In Titles and Headings</td>
</tr>
<tr>
<td>anti-bicyclo[3.2.1]octan-8-amine</td>
</tr>
<tr>
<td>cis-1,2-dichloroethene</td>
</tr>
<tr>
<td>d-camphor</td>
</tr>
<tr>
<td>dl-2-aminopropanoic acid</td>
</tr>
<tr>
<td>(E)-diphenylhydrazine</td>
</tr>
<tr>
<td>endo-2-chlorobicyclo[2.2.1]-heptane</td>
</tr>
<tr>
<td>(+)-erythro-2-amino-3-methylpentanoic acid</td>
</tr>
<tr>
<td>erythro-β-hydroxyaspartic acid</td>
</tr>
<tr>
<td>exo-5,6-dimethylendo-bicyclo[2.2.2]octan-2-ol</td>
</tr>
<tr>
<td>L-theo-2,3-dichlorobutyric acid</td>
</tr>
<tr>
<td>meso-tartaric acid</td>
</tr>
<tr>
<td>(1R*,3S*)-1-bromo-3-chlorocyclohexane</td>
</tr>
<tr>
<td>rel-(1R,3R)-1-bromo-3-chlorocyclohexane</td>
</tr>
<tr>
<td>(5S,2,3-dihydroxypropanoic acid</td>
</tr>
<tr>
<td>sn-glycerol 1-(dihydrogen phosphate)</td>
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<tr>
<td>syn-7-methylbicyclo[2.2.1]-heptene</td>
</tr>
<tr>
<td>trans-cisoid-trans-perhydrophenanthrene</td>
</tr>
<tr>
<td>(Z)-5-chloro-4-pentenoic acid</td>
</tr>
<tr>
<td>(1Z,4E)-1,2,4,5-tetrachloro-1,4-pentadiene</td>
</tr>
</tbody>
</table>
Use italic letters within square brackets in names of polycyclic aromatic compounds.

- dibenz[a,j]anthracene
- dibenzo[c,g]phenanthrene
- dicyclobuta[de,ii]naphthalene
- 1H-benzo[de]naphthacene
- indeno[1,2-a]indene

**Syllabic Portion of Chemical Names**

Multiplying affixes are integral parts of the chemical name; they are set in roman type and are always closed up to the rest of the name (without hyphens). Use hyphens only to set off intervening locants or descriptors. Use enclosing marks (parentheses, brackets, or braces) to ensure clarity or to observe other recommended nomenclature conventions. Multiplying prefixes include the following:

- hemi, mono, di, tri, tetra, penta, hexa, hepta, octa, ennea, nona, deca, deka, undeca, dodeca, etc.
- semi, uni, sesqui, bi, ter, quadri, quater, quinque, sexi, septi, octi, novi, deci, etc.
- bis, tris, tetrakis, pentakis, hexakis, heptakis, octakis, nonakis, decakis, etc.

<table>
<thead>
<tr>
<th>Chemical Name</th>
<th>Capitalized Form</th>
</tr>
</thead>
<tbody>
<tr>
<td>3,4′-bi-2-naphthol</td>
<td>pentachloroethene</td>
</tr>
<tr>
<td>2,2′-bipyridine</td>
<td>3,4,5,6-tetrabromo-o-cresol</td>
</tr>
<tr>
<td>bis(benzene)chromium(0)</td>
<td>tetrakis(hydroxymethyl)methane</td>
</tr>
<tr>
<td>1,4-bis(3-bromo-1-oxopropyl)piperazine</td>
<td>tri-sec-butylamine</td>
</tr>
<tr>
<td>1,3-bis(diethylamino)propane</td>
<td>triethyl phosphate</td>
</tr>
<tr>
<td>di-tert-butyl malonate</td>
<td>tris(amine)</td>
</tr>
<tr>
<td>dichloride</td>
<td>2,3,5-tris(aziridin-1-yl)-p-benzoquinone</td>
</tr>
<tr>
<td>1,2-ethanediol</td>
<td>tri(ethylenediamine)cadmium</td>
</tr>
<tr>
<td>hemihydrate</td>
<td>dihydroxide</td>
</tr>
<tr>
<td>hexachlorobenzene</td>
<td></td>
</tr>
<tr>
<td>2,4,6,8-nonanetetraone</td>
<td></td>
</tr>
</tbody>
</table>

**Capitalization of Chemical Names**

Chemical names are not capitalized unless they are the first word of a sentence or are part of a title or heading. Then, the first letter of the syllabic portion is capitalized, not the locant, stereoisomer descriptor, or positional prefix. Table 12-1 presents examples of simple chemical names and their capitalization. Table 12-2 presents chemical names that include locants and descriptors.

Some reaction names are preceded by element symbols; they may be used as nouns or adjectives. When they are the first word of a sentence or appear in titles
and headings, capitalize the first letter of the word. Do not italicize the element symbol.

N-Oxidation of the starting compounds yielded compounds 3–10.

N-Benzoylated amines undergo hydroxylation when incubated with yeast.

Preparation of S-Methylated Derivatives

O-Substituted Structural and Functional Analogues

**Punctuation in Chemical Names**

➤ Use commas between numeral locants, chemical element symbol locants, and Greek locants, with no space after the comma. When a single locant consists of a numeral and a Greek letter together with no space or punctuation, the numeral precedes the Greek letter. When the Greek letter precedes the numeral, they indicate two different locants and should be separated by a comma. For example, α,2 denotes two locants; 1α is viewed as one locant.

(6α,11β,16α)-6-fluoro-16-methylpregna-1,4-diene
β,4-dichlorocyclohexanepropionic acid
1,2-dinitrobutane
N,N-dimethylacetamide
2,3,3a,4-tetrahydro-1H-indole

➤ Use hyphens to separate locants and configurational descriptors from each other and from the syllabic portion of the name.

α-ketoglutaric acid
2-benzyloibenzoic acid
1,4-bis(2-ethylhexyl) sulfosuccinate
3-chloro-4-methylbenzoic acid
cis-dichloroethylene
d-arabinose
(1,4-dioxaspiro[4.5]dec-2-ylmethyl) guanidine
(E)-2-(3,7-dimethyl-2,6-octadienyl)-1,4-benzenediol
N-hydroxy-N-nitrosobenzeneamine
N-methylmethanamine
4-O-β-p-galactopyranosyl-p-fructose
tetrahydro-3,4-dipiperonyl-2-furanol
trans-2-bromocyclopentanol

➤ Do not use hyphens to separate the syllables of a chemical name unless the name is too long to fit on one line. Appendix 12-1 is a list of prefixes, suffixes, roots, and some complete words hyphenated as they would be at the end of a line.
**Specialized Groups of Chemicals**

**Polymers**

Polymer names are often one or two words in parentheses following the prefix “poly”. “Poly” is a syllabic prefix, not a descriptor, and thus is set in roman type. Here is a short list of correctly formatted names of frequently cited polymers. (These names are not necessarily IUPAC or CA index preferences.)

<table>
<thead>
<tr>
<th>Polymer Name</th>
<th>Full Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>nylon-6</td>
<td>poly(isobutyl methacrylate)</td>
</tr>
<tr>
<td>nylon-6,6</td>
<td>polyisobutylene</td>
</tr>
<tr>
<td>polyacrylamide</td>
<td>polyisoprene</td>
</tr>
<tr>
<td>poly(acrylic acid)</td>
<td>poly(methacrylic acid)</td>
</tr>
<tr>
<td>polyacrylonitrile</td>
<td>poly(methyl acrylate)</td>
</tr>
<tr>
<td>polyamide</td>
<td>poly(methyl methacrylate)</td>
</tr>
<tr>
<td>poly(aryl sulfone)</td>
<td>poly(methylene)</td>
</tr>
<tr>
<td>polybutadiene</td>
<td>poly(N,N'-hexamethylenediamide)</td>
</tr>
<tr>
<td>1,2-polybutadiene</td>
<td>poly(oxy-1,4-phenylene)</td>
</tr>
<tr>
<td>1,4-polybutadiene</td>
<td>poly(oxyethylene)</td>
</tr>
<tr>
<td>poly(butyl acrylate)</td>
<td>poly(oxymethylene)</td>
</tr>
<tr>
<td>poly(butyl methacrylate)</td>
<td>poly(phenylene ether)</td>
</tr>
<tr>
<td>poly(n-butyl methacrylate)</td>
<td>poly(phenylene oxide)</td>
</tr>
<tr>
<td>poly(butylene terephthalate)</td>
<td>poly(phenylene sulfide)</td>
</tr>
<tr>
<td>polycarbonate</td>
<td>polypropylene</td>
</tr>
<tr>
<td>polychloroprene</td>
<td>poly(propylene glycol)</td>
</tr>
<tr>
<td>poly(N,N-dimethylacrylamide)</td>
<td>polystyrene</td>
</tr>
<tr>
<td>poly(dimethylsiloxane)</td>
<td>polysulfide</td>
</tr>
<tr>
<td>polyester</td>
<td>polysulfone</td>
</tr>
<tr>
<td>poly(ether imide)</td>
<td>poly(tetrafluoroethylene)</td>
</tr>
<tr>
<td>poly(ether ketone)</td>
<td>poly(tetramethylene oxide)</td>
</tr>
<tr>
<td>poly(ether sulfone)</td>
<td>poly(thiocarbonate)</td>
</tr>
<tr>
<td>poly(ethyl acrylate)</td>
<td>polyurethane</td>
</tr>
<tr>
<td>poly(ethyl methacrylate)</td>
<td>poly(vinyl acetate)</td>
</tr>
<tr>
<td>polyethylene</td>
<td>poly(vinyl alcohol)</td>
</tr>
<tr>
<td>poly(ethylene adipate)</td>
<td>poly(vinyl butyral)</td>
</tr>
<tr>
<td>poly(ethylene glycol)</td>
<td>poly(vinyl chloride)</td>
</tr>
<tr>
<td>poly(ethylene oxide)</td>
<td>poly(vinyl ether)</td>
</tr>
<tr>
<td>poly(ethylene terephthalate)</td>
<td>poly(vinyl trichloroacetate)</td>
</tr>
<tr>
<td>polyformaldehyde</td>
<td>poly(vinylidene chloride)</td>
</tr>
<tr>
<td>polyimidazole</td>
<td>poly(vinylpyrrolidone)</td>
</tr>
<tr>
<td>polyimide</td>
<td>povidone</td>
</tr>
</tbody>
</table>

In text, keep polymer names lowercase. As the first word of a sentence and in titles or headings, capitalize only the first letter of the polymer name.

New Uses for Poly(ethylene terephthalate)
Poly(vinyl chloride) is a less useful polymer than poly(ethylene glycol).

Reactions of Poly(methyl methacrylate)

➤ In copolymer nomenclature, descriptive lowercase italic infixes may be used. These include alt, blend, block (or b), co, cross, graft (or g), inter, per, stat, and ran.

- polybutadiene-\textit{graft}-\{polystyrene:poly(methyl methacrylate)\}
- poly(\textit{cross}-butadiene)
- poly[\textit{cross}-\{ethyl acrylate\}-\textit{inter}-polybutadiene]
- poly(ethylene-\textit{alt}-carbon monoxide)
- polyisoprene-\textit{blend}-polystyrene
- poly[\{methyl methacrylate\}-\textit{b}-\{styrene-\textit{co}-butadiene\}]
- poly[\{methyl methacrylate\}-\textit{co}-styrene]
- polystyrene-\textit{block}-polybutadiene
- poly(styrene-\textit{co}-butadiene)
- poly(styrene-\textit{g}-acrylonitrile)
- poly(vinyl trichloroacetate)-\textit{cross}-polystyrene

**Saccharides**

Abbreviations for the major monosaccharides are presented in Table 12-3.

➤ Designation of the bond between two monosaccharides should specify the first residue, its anomeric configuration (α or β), the position of attachment on both sugar residues, and the second residue. Additional locants and configurational descriptors may be present but are not required. A number of variations may be used.

| Gal\(\beta_{1\rightarrow4}\)Glc | Gal\(\beta_{1–4}\)Glc | Gal\(\beta_{1,4}\)Glc |
| Gal\(\beta(1\rightarrow4)\)Glc | Gal\(\beta(1–4)\)Glc | Gal\(\beta(1,4)\)Glc |

**Table 12-3. Abbreviations for Major Monosaccharides**

<table>
<thead>
<tr>
<th>Saccharide</th>
<th>Abbreviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>arabinose</td>
<td>Ara</td>
</tr>
<tr>
<td>fucose</td>
<td>Fuc</td>
</tr>
<tr>
<td>galactose</td>
<td>Gal</td>
</tr>
<tr>
<td>N-acetylgalactosamine</td>
<td>GalNAc</td>
</tr>
<tr>
<td>glucose</td>
<td>Glc</td>
</tr>
<tr>
<td>N-acetylglucosamine</td>
<td>GlcNAc</td>
</tr>
<tr>
<td>glucuronic acid</td>
<td>GlcA</td>
</tr>
<tr>
<td>mannose</td>
<td>Man</td>
</tr>
<tr>
<td>N-acetyleneuraminic acid</td>
<td>Neu5Ac</td>
</tr>
<tr>
<td>N-glycoloylneuraminic acid</td>
<td>Neu5Gc</td>
</tr>
<tr>
<td>rhamnose</td>
<td>Rha</td>
</tr>
<tr>
<td>xylose</td>
<td>Xyl</td>
</tr>
</tbody>
</table>
For larger oligosaccharides, use parentheses or brackets for branched residues:

\[ \text{Man}_\alpha 1\to 6(\text{Man}_\alpha 1\to 3)\text{Man}_\beta 1\to 4\text{GlcNAc}_\beta 1\to 4(\pm\text{Fuc}_\alpha 1\to 6)\text{GlcNAc} \]

\[ \text{Man}(1\to 6)[\text{Man}(1\to 3)\text{Man}(1\to 4)\text{GlcNAc}_\beta(1\to 4)(\pm\text{Fuc}(1\to 6))\text{GlcNAc} \]

**Nucleic Acids**

Table 12-4 presents the standard abbreviations for nucleic acids.

By convention, numbering of the bases is unprimed and numbering of the sugars is primed. A nucleic acid polymer typically has the phosphate group attached to the 5’ position of the first nucleotide (the 5’ end), and the other end terminates in a hydroxyl group at the 3’ position of the sugar of the last nucleotide (the 3’ end). By convention, nucleotide sequences are almost always read and presented in the 5’ to 3’ direction. The sequence may be presented in unbroken form or in evenly spaced blocks.

5’-TAGCTAAACCGTTTATACGTCGTC-3’

5’-TAGCTAACCC GTTTT AGCGT CGTC-3’

Complementary base pairs are joined by hydrogen bonds and are best represented by a centered dot: dA·dT and dG·dC are the canonical pairings in double-stranded DNA, although alternate pairings, DNA·RNA hybrids, triplexes, and other variations may occur.

**Table 12-4. Abbreviations for Nucleic Acids**

<table>
<thead>
<tr>
<th>Base</th>
<th>Sugar</th>
<th>Nucleoside&lt;sup&gt;a&lt;/sup&gt; (base + sugar)</th>
<th>Abbreviation for Nucleoside Monophosphate&lt;sup&gt;b&lt;/sup&gt;</th>
<th>Nucleoside Diphosphate</th>
<th>Nucleoside Triphosphate</th>
</tr>
</thead>
<tbody>
<tr>
<td>adenine</td>
<td>ribose</td>
<td>adenosine, A</td>
<td>AMP</td>
<td>ADP</td>
<td>ATP</td>
</tr>
<tr>
<td>cytosine</td>
<td>ribose</td>
<td>cytidine, C</td>
<td>CMP</td>
<td>CDP</td>
<td>CTP</td>
</tr>
<tr>
<td>guanine</td>
<td>ribose</td>
<td>guanosine, G</td>
<td>GMP</td>
<td>GDP</td>
<td>GTP</td>
</tr>
<tr>
<td>uracil</td>
<td>ribose</td>
<td>uridine, U</td>
<td>UMP</td>
<td>UDP</td>
<td>UTP</td>
</tr>
</tbody>
</table>

<sup>a</sup>Other nucleosides may occur (e.g., inosine, I, or xanthosine, X), but those listed are the canonical building blocks of nucleic acids and need never be defined. N may be used for an unspecified nucleoside or a mixture of all four (i.e., dNTPs were added to the reaction mixture).

<sup>b</sup>A nucleoside monophosphate is also known as a nucleotide.

<sup>c</sup>Thymidine consists of thymine + deoxyribose by definition and is abbreviated dT by definition; deoxythymidine would imply a different compound lacking another oxygen.
Amino Acids

The abbreviations of the essential 20 amino acids are listed in Table 12-5; these abbreviations do not need to be defined. In analytical situations, undifferentiated mixtures of aspartic acid/asparagine (Asx, B) or glutamic acid/glutamine (Glx, Z) may occur.

For amino acids other than the essential 20, three-letter abbreviations may be used and defined at their first appearance.

- homocysteine: Hcy
- hydroxyproline: Hyp
- norvaline: Nva
- ornithine: Orn

Three-letter amino acid abbreviations may be preceded by a configurational designator, d or l, set in small capital letters.

Always capitalize the three-letter and one-letter abbreviations for amino acids.

In sequences of amino acids, separate the three-letter abbreviations with hyphens.

Pro-Gln-Ile-Ala

Table 12-5. Abbreviations for Amino Acids

<table>
<thead>
<tr>
<th>Amino Acid</th>
<th>Three-Letter Abbreviation</th>
<th>One-Letter Abbreviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>alanine</td>
<td>Ala</td>
<td>A</td>
</tr>
<tr>
<td>arginine</td>
<td>Arg</td>
<td>R</td>
</tr>
<tr>
<td>asparagine</td>
<td>Asn</td>
<td>N</td>
</tr>
<tr>
<td>aspartic acid</td>
<td>Asp</td>
<td>D</td>
</tr>
<tr>
<td>cysteine</td>
<td>Cys</td>
<td>C</td>
</tr>
<tr>
<td>glutamic acid</td>
<td>Glu</td>
<td>E</td>
</tr>
<tr>
<td>glutamine</td>
<td>Gln</td>
<td>Q</td>
</tr>
<tr>
<td>glycine</td>
<td>Gly</td>
<td>G</td>
</tr>
<tr>
<td>histidine</td>
<td>His</td>
<td>H</td>
</tr>
<tr>
<td>isoleucine</td>
<td>Ile</td>
<td>I</td>
</tr>
<tr>
<td>leucine</td>
<td>Leu</td>
<td>L</td>
</tr>
<tr>
<td>lysine</td>
<td>Lys</td>
<td>K</td>
</tr>
<tr>
<td>methionine</td>
<td>Met</td>
<td>M</td>
</tr>
<tr>
<td>phenylalanine</td>
<td>Phe</td>
<td>F</td>
</tr>
<tr>
<td>proline</td>
<td>Pro</td>
<td>P</td>
</tr>
<tr>
<td>serine</td>
<td>Ser</td>
<td>S</td>
</tr>
<tr>
<td>threonine</td>
<td>Thr</td>
<td>T</td>
</tr>
<tr>
<td>tryptophan</td>
<td>Trp</td>
<td>W</td>
</tr>
<tr>
<td>tyrosine</td>
<td>Tyr</td>
<td>Y</td>
</tr>
<tr>
<td>valine</td>
<td>Val</td>
<td>V</td>
</tr>
</tbody>
</table>
Do not use abbreviations for individual amino acids in running text. Selective labeling of arginine and serine made it possible to monitor the kinetics of folding of the individual residues.

Position numbers may follow one- or three-letter abbreviations or spelled-out names and may be closed up, hyphenated, spaced, or superscripted. Designation of a mutation includes the original amino acid, the position number, and the new amino acid:

- A134V
- Ala134Val
- alanine-134 → valine

**Combinatorial Compounds**

Combinatorial libraries are described by generic representations, which consist of a generic structure together with one or more lists of substituents. The position of substituents is indicated by superatoms in the generic structure.

Superatoms are designated by roman letters: R for any set of substituents or residues, for example, or Ar for a list of aromatic substituents. Superatoms may be distinguished by the addition of designation digits, typically a subscript following the superatom: R_<sub>A</sub>, R_<sub>B</sub>, and R_<sub>C</sub> could specify the residue of reagents A, B, and C.

Subscript numbers are generally used to indicate the order in which residues were introduced to the reaction scheme: R<sub>1</sub>, R<sub>2</sub>, R<sub>3</sub>, and so on.

The *Journal of Combinatorial Chemistry* recommends the use of ChemSet notation, in which a structure number is followed by the reagent sets associated with it. The structure number is typeset in bold, and the reagent sets are set in italics and enclosed in curly brackets.

- \[ \text{1\{1–5\} + 2\{1–6\} + 4\{1–4\} \rightarrow 5\{1–5,1–4,1–6\} } \]
- \[ 4\{1–5,1–4,1–6\} \]

The composition of a final library can be described in terms of mixtures or separate products. An uppercase X is used to indicate products mixed; an uppercase O is used to indicate products separate.

- \[ 4\{X,X,O\} \]
- \[ 4\{X 1–5,X 1–4,O 1–6\} \]
- \[ 4\{O,O,O\} \]
- \[ 4\{O 1–5,O 1–4,O 1–6\} \]

Additional information on the representation of combinatorial chemistry is given in Appendix 12-2.
## APPENDIX 12-1

### End-of-Line Hyphenation of Chemical Names

This appendix contains a list of prefixes, suffixes, roots, and some complete words hyphenated as they would be at the end of a line. To hyphenate a chemical name such as

5-(2-chloroethyl)-9-(diaminomethyl)-2-anthracenol

look up each syllable that is to be hyphenated in the list. Also, chemical names can be broken after hyphens that are integral in their names. Follow other standard rules for hyphenation of regular words; for example, try to leave at least three characters on each line. Thus, the example given could be hyphenated as follows:

5-(2-chlo-ro-eth-yl)-9-(di-ami-no-meth-yl)-2-anth-ra-cenol

Most desk dictionaries contain the names of common chemicals; they also give end-of-line hyphenation.

<table>
<thead>
<tr>
<th>Prefix/Suffix</th>
<th>Prefix/Suffix</th>
<th>Prefix/Suffix</th>
</tr>
</thead>
<tbody>
<tr>
<td>ace-naph-tho</td>
<td>ac-ry-lo</td>
<td>azo</td>
</tr>
<tr>
<td>ace-tal</td>
<td>ad-i-po-yl</td>
<td>benz-ami-do</td>
</tr>
<tr>
<td>acet-al-de-hyde</td>
<td>al-kyl</td>
<td>ben-zene</td>
</tr>
<tr>
<td>acet-amide</td>
<td>al-lyl</td>
<td>benz-hy-dryl</td>
</tr>
<tr>
<td>acet-ami-do</td>
<td>ami-di-no</td>
<td>ben-zy-l</td>
</tr>
<tr>
<td>acet-amin-o-phen</td>
<td>amide</td>
<td>ben-zy-l-i-dene</td>
</tr>
<tr>
<td>acet-an-i-lide</td>
<td>ami-do</td>
<td>bi-cy-clo</td>
</tr>
<tr>
<td>ace-tate</td>
<td>amine</td>
<td>bo-ryl</td>
</tr>
<tr>
<td>ac-et-azol-amide</td>
<td>ami-no</td>
<td>bro-mide</td>
</tr>
<tr>
<td>ace-tic</td>
<td>am-mine</td>
<td>bro-mo</td>
</tr>
<tr>
<td>ace-to</td>
<td>am-mo-nio</td>
<td>bu-tane</td>
</tr>
<tr>
<td>ace-to-ace-tic</td>
<td>am-mo-ni-um</td>
<td>bu-ten-yl</td>
</tr>
<tr>
<td>ace-tone</td>
<td>an-thra</td>
<td>bu-tyl</td>
</tr>
<tr>
<td>ace-to-ni-trile</td>
<td>an-thra-cene</td>
<td>bu-tyl-ene</td>
</tr>
<tr>
<td>ace-tyl</td>
<td>an-thra-ce-no</td>
<td>bu-tyl-i-dene</td>
</tr>
<tr>
<td>acet-y-late</td>
<td>an-thryl</td>
<td>car-ba-mate</td>
</tr>
<tr>
<td>acet-y-lene</td>
<td>ar-se-nate</td>
<td>car-bam-ic</td>
</tr>
<tr>
<td>acro-le-in</td>
<td>ar-si-no</td>
<td>car-ba-mide</td>
</tr>
<tr>
<td>ac-ryl-am-ide</td>
<td>aryl</td>
<td>carb-an-ion</td>
</tr>
<tr>
<td>ac-ry-late</td>
<td>az-i-do</td>
<td>car-ba-ryl</td>
</tr>
<tr>
<td>acryl-ic</td>
<td>azi-no</td>
<td></td>
</tr>
<tr>
<td>Compound</td>
<td>Abbreviation</td>
<td>Compound</td>
</tr>
<tr>
<td>-----------</td>
<td>---------------</td>
<td>-----------</td>
</tr>
<tr>
<td>car-ba-zole</td>
<td>for-mic</td>
<td>iso-pro-pyl</td>
</tr>
<tr>
<td>car-bi-nol</td>
<td>for-my-l</td>
<td>mer-cu-to</td>
</tr>
<tr>
<td>car-bol-ic</td>
<td>for-my-l</td>
<td>mer-cu-ric</td>
</tr>
<tr>
<td>car-bon-ate</td>
<td>fu-ran</td>
<td>meth-an-ami-do</td>
</tr>
<tr>
<td>car-bon-ic</td>
<td>ger-my-l</td>
<td>meth-ane</td>
</tr>
<tr>
<td>car-bo-ni-um</td>
<td>gua-ni-di-no</td>
<td>meth-ano</td>
</tr>
<tr>
<td>car-bon-yl</td>
<td>gua-nyl</td>
<td>meth-yl</td>
</tr>
<tr>
<td>car-box-ami-do</td>
<td>halo</td>
<td>meth-yl-ate</td>
</tr>
<tr>
<td>car-boxy</td>
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phos-phite
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phos-phor-anyl
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phos-pho-lip-id
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pyr-role
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qui-none
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stan-nite
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stan-nyl
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sty-reno
sty-ryl
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sul-fe-no
sul-fe-nyl
sul-fide
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sul-fi-no
sul-fi-nyl
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sul-fon-ami-do
sul-fone
sul-fon-ic
sul-fo-nio
sul-fo-nyl
sul-fu-ric
sul-fu-rous
sul-fu-ryl
tet-ra
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thio-phene
thi-oxy
thi-oxy
tol-u-ene
tol-u-ide
tol-yl
tri-a-zine
tri-a-zole
tri-yl
urea
ure-ide
ure-ido
uric
vi-nyl
vi-nyl-i-dene
xan-thene
xan-tho
xy-lene
xy-li-dine
xy-lyl
xy-li-din-yl
yl-i-dene
Combinatorial chemistry entails the reaction of \textit{sets} of reagents to produce \textit{sets} or \textit{libraries} of products in numbers up to the size of each reagent set multiplied together. Thus 5 reagents A, plus 4 reagents B, plus 6 reagents C could prepare $5 \times 4 \times 6$, or 120 products ABC. The unique feature of this strategy is the ability to efficiently prepare very large numbers of compounds—a so-called \textit{combinatorial library}. The challenges in describing combinatorial chemistry consist of concisely but accurately reporting the constituents and form of such a compound collection.

The individual products of combinatorial chemistry are called \textit{members}. The distinction between a member and a \textit{compound} is important and is based on the respective level of characterization. A compound will meet the typical standards for reporting new chemical structures; a member will fall short of that standard. In fact, a member may, in principle, simply be \textit{expected} to be present in a library, especially for large libraries, and those that consist of mixtures rather than discrete samples of members.

The structural representation of combinatorial chemistry consists of a \textit{generic structure} plus a list of \textit{substituents} that may be present in that structure.

The generic structure is very similar to a typical structural formula with the addition of special notation to indicate the potential for variable substitution at certain parts of the molecule.

The position of variable substituents on a generic structure is indicated by \textit{superatoms}, such as the R designation. In a combinatorial library, R need not simply designate an alkyl radical but is conventionally used to represent any set of substituents or \textit{residues}. The residues R typically define those portions of reagents or building blocks that are found in the final product of the synthesis and that vary among library members. Particular superatoms may more precisely define the composition of a library, such as Ar for a list of aromatic substituents.

To distinguish superatoms within a generic structure, it is typical to use additional designation digits. Thus $R_A$, $R_B$, and $R_C$ could specify the residue of reagents A, B, and C in our example. The position of the additional digit has
not been standardized but may be typically added as a subscript following the superatom.

The designation digit may usefully convey additional information beyond the simple differentiation of superatoms. For instance, R₁, R₂, R₃, and so on may indicate the order in which these residues were introduced to the reaction scheme. Alternatively, Rₓ or Rₒ make use of the pool designations X and O (see the section “ChemSet Notation”) to concisely describe library composition in a generic structure.

It is often possible to draw multiple generic structures for a combinatorial library. Care should be taken in the choice of the appropriate structure, taking into account the purpose for the structure. Often the maximum common substructure is a good choice, but other structures may better illustrate structure–activity relationships or the synthetic potential of a combinatorial reaction strategy. The relationship between residue and reagent or product should be defined. This may be conveniently shown in the generic reaction scheme; see Figure 12A-1.

A typical feature of combinatorial synthesis is the use of techniques that facilitate the isolation of products and intermediates. The most common example is the attachment to a solid support, such as a polymer bead, to allow isolation by simple filtration (solid-phase chemistry). A variety of solid and soluble supports have been developed. These may be attached to either the products or the reagents of a library.

Such supports can be dealt with in generic reaction schemes as a special type of superatom. Often, a pictorial representation is used. A polymer bead may be conveniently represented by an s orbital in common chemistry software packages. Few standards have been developed for the representation of other supports, but a filled structure designates a solid support and an open structure may be used for a soluble support.

**ChemSet Notation**

A convenient descriptive notation for combinatorial libraries (recommended by the *Journal of Combinatorial Chemistry*) is the ChemSet terminology.

A ChemSet is denoted by a structure number followed by the reagent sets associated with that structure. Thus the combinatorial library with 120 products could be described as follows, where the numbers in curly brackets define the reagents which were used to prepare that library; see Figure 12A-1.

\[ 5 \{1–5,1–6,1–4\} \]

The synthetic scheme to prepare such a library may also be described in terms of ChemSets:

\[ 1\{1–5\} + 2\{1–6\} + 4\{1–4\} \rightarrow 5\{1–5,1–6,1–4\} \]

The composition of the final library may consist of a mixture of all members, or as a collection of discrete product samples, or as a set of smaller pools. An exten-
The ACS Style Guide

The useful designations X and O indicate respectively, “products mixed” and “products separate”. Thus, the library 5{X 1–5,X 1–6,O 1–4} is a set of 6 pools, each with 20 members deriving from a single reagent from set 4, since the O indicates that the six individual product mixtures were kept separate from one another after adding reagents 4. In contrast, 5{O 1–5,O 1–4,O 1–6} represents 120 discrete product samples, also called parallel synthesis, since the O for each set indicates that all products were kept separate at each stage.

If all of a given set of reagents have been used in a given pool, then the number for that set may be omitted. Thus, 5{X,X,O} and 5{O,O,O} accurately describe the composition of the above libraries. However, if a subset of possible reagents have been used, this must be indicated using the numerical list format, e.g., 5{X 1–6,O 1–2,3}.

Figure 12A-1. Combinatorial reaction scheme and ChemSet notation.

Chemical substances, their syntheses, the determination of their properties, and their applications are the core of chemistry and the main occupation of chemists. In their communications, chemists represent chemical substances by structural diagrams, names, molecular formulas, codes, and identification numbers. One of the most frequently used identification numbers is the CAS Registry Number. Today, CAS Registry Numbers are often used to identify chemical substances in handbooks, indexes, databases, and inventories, and even on many commercial product labels.

The CAS Chemical Registry System is a computer-based system that uniquely identifies chemical substances on the basis of their molecular structures. Begun originally in 1965 to support indexing for *Chemical Abstracts* (CA), the CAS Chemical Registry System now serves not only as a support system for identifying substances within Chemical Abstracts Service operations but also as an international resource for chemical substance identification by scientists, industry, and regulatory bodies. The CAS Registry provides a means of bridging the many differences in systematic, generic, proprietary, and trivial substance names that may be used to identify a single substance.

The CAS Chemical Registry System database is the largest collection of information on naturally occurring and synthetic chemical substances in the world, including organic compounds, inorganic compounds, organometallics, metals, polymers, coordination compounds, alloys, elements, isotopes, nuclear particles, proteins, nucleic acids, and minerals. By the end of 2005, the CAS Chemical Registry System contained records for more than 27 million organic and inorganic substances, with new records added at the rate of some 5000 per day. A running total of registered substances can be found on the CAS Web site at http://www.cas.org/cgi-bin/regreport.pl.

The database contains CAS Registry Numbers, structures, and names for substances reported in the chemical literature covered in CA, in addition to substances registered from special collections, for governmental and industrial organizations, and for individual requesters. CAS Registry Numbers are also assigned to sequences such as DNA and proteins.

CAS Registry Numbers are assigned in sequential order as substances are entered into the CAS Chemical Registry System database for the first time; the numbers have no chemical significance. CAS Registry Numbers link the molecular structure diagram, systematic CA index name, synonyms, molecular formula,
and other identifying information for each substance. Because CAS Registry Numbers are independent of the many different systems of chemical nomenclature, they can bridge these systems and link often unrecognized synonymous names.

A format was developed using hyphens to make the numbers easier to read and to recognize. A CAS Registry Number includes up to nine digits that are separated into three parts by hyphens. The first part, starting from the left, has up to six digits, the second part has two digits, and the final part is a single check digit to verify the validity of the total number (e.g., 7732-18-5 for water).

Within the registry system, each substance is assigned a separate CAS Registry Number. For example, each salt of an acid receives a distinct number, and an ion receives a number different from that of the neutral compound.

CAS Registry Numbers are included in the printed *Chemical Abstracts* chemical substance and formula indexes and in the CAS databases. The full set of CAS Chemical Registry System database information—structures, names, formulas, and ring data—is available for search and display through STN International, SciFinder, and other CAS search services. CAS Registry information is also available in CAS databases offered by other online system vendors.

In addition to their inclusion in the CAS databases, CAS Registry Numbers are used in many public and private databases. Many handbooks, guides, and other reference works include CAS Registry Numbers and provide special indexes that allow the reader to find the proper place in the text without first having to identify the full name of the substance. The reader benefits because the full name may differ from handbook to handbook.

CAS Registry Numbers are also widely used as standard identifiers for chemical substances in many of the commercial chemical inventories of governmental regulatory agencies, such as the Toxic Substances Control Act (TSCA) Inventory in the United States, the European Inventory of Existing Commercial Chemical Substances (EINECS), and the Canadian Domestic and Non-Domestic Substance Lists (DSL/NDSL).

Whenever a chemical substance is sold, transported, imported, exported, reported to a regulatory agency, or disposed of, a CAS Registry Number is probably involved.
This chapter presents a quick reference guide for the use of typefaces (roman, italic, and bold), Greek letters, superscripts and subscripts, and special symbols that are commonly used in chemistry. Appendix 13-1 presents the symbols for commonly used physical quantities.


Some books and journals follow IUPAC recommendations for representations of various chemical conventions. Some specify the use of ISO standards. Others are less stringent as long as the manuscript is consistent in usage within itself. Always consult the author guidelines.
Subatomic Particles and Quanta

➤ Use lowercase Latin or Greek letters for abbreviations for subatomic particles.

- alpha particle \( \alpha \)
- beta particle \( \beta \)
- deuteron \( d \)
- electron \( e \)
- helion \( h \)
- muon \( \mu \)
- neutron \( n \)
- photon \( \gamma \)
- pion \( \pi \)
- proton \( p \)
- neutrino \( \nu_e \)
- triton \( t \)

➤ Indicate electric charges with the appropriate superscript (+, −, or 0).

\[ n^0 \]
\[ e^+ \]
\[ e^- \]
\[ \pi^\pm \]

If the symbols \( p \) and \( e \) are used without indication of charge, they refer to positive proton and negative electron, respectively.

Electronic Configuration

➤ Denote electron shells with the uppercase roman letters K, L, M, and N.

➤ Name electron subshells and atomic orbitals with the lowercase roman letters s, p, d, and f. Write principal energy levels 1–7 on the line and to the left of the letter; give the number of electrons in the orbital as a superscript to the right of the letter. Specify orbital axes with italic subscripts.

- 7s electron
- 5f\(^2\) ions
- 5f orbital
- 6d orbital
- sp\(^3\) hybrid orbital
- f\(^6\)–3ds\(^2\) configuration

The ground state of boron is 1s\(^2\)2s\(^2\)2p\(_x\)^12p\(_y\)^02p\(_z\)^0.

The valence-shell configuration of nitrogen is 2s\(^2\)2p\(_x\)^12p\(_y\)^12p\(_z\)^1.

The electronic configuration of potassium is 1s\(^2\)2s\(^2\)2p\(^6\)3s\(^2\)3p\(^6\)4s\(^1\).

The valence-electron configuration is described by 5d\(^{10}\)6s\(^1\).

➤ Use Greek letters for some bonding orbitals and the bonds they generate.

- \( \pi \) bond
- \( \sigma \) orbital
- \( \sigma^* \) orbital
Name the electronic states of atoms with the uppercase roman letters S, P, D, F, G, H, I, and K, corresponding to quantum numbers \( l = 0 \text{–} 7 \). Use the corresponding lowercase letters to indicate the orbital angular momentum of a single electron. The left superscript is the spin multiplicity; the right subscript is the total angular momentum quantum number \( J \).

\[
\begin{align*}
2S \quad & 4P_{1/2} \\
2S \quad & 4P_{1/2} \\
8F_{1/2} \quad & 8G_{1/2} \\
8F_{1/2} \quad & 8G_{1/2}
\end{align*}
\]

Name the electronic states of molecules with the uppercase roman letters A, B, E, and T; the ground state is X. Use the corresponding lowercase letters for one-electron orbitals. A tilde (~) is added for polyatomic molecules. The subscripts describe the symmetry of the orbital.

\[
\begin{align*}
2A & \quad 2a_{1g} \\
2A_1 \quad & 2a_{2g} \\
A_2 \quad & 3B_1 \\
\tilde{a} & \quad 3b_1 \\
E & \quad E_g \\
E & \quad E_{2g} \\
e & \quad e_g \\
t & \quad t_{2g}
\end{align*}
\]

**Chemical Elements and Formulas**

Write the names of the chemical elements in roman type and treat them as common nouns.

- calcium
- francium
- oxygen
- californium
- helium
- seaborium
- carbon
- hydrogen
- uranium

Write the symbols for the chemical elements in roman type with an initial capital letter.

- Ca
- Es
- H
- Sg
- Cf
- Fr
- O
- U
- C
- He

The complete list of chemical elements and symbols is given in Table 13-1.

Even when symbols are used, the element’s name is pronounced. Therefore, choose the article (a or an) preceding the element symbol to accommodate the pronunciation of the element name. (This usage does not apply to isotopes, as described in the section on isotopes.)

- a Au electrode (pronounced “a gold electrode”)
- a N-containing compound (pronounced “a nitrogen-containing compound”)
- a He–Ne laser (pronounced “a helium–neon laser”)

Chapter 13: Conventions in Chemistry ➤ 257
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<td>Gadolinium</td>
<td>Gd</td>
<td>64</td>
<td>157.25(3)</td>
<td>g</td>
</tr>
<tr>
<td>Gallium</td>
<td>Ga</td>
<td>31</td>
<td>69.723(1)</td>
<td></td>
</tr>
<tr>
<td>Germanium</td>
<td>Ge</td>
<td>32</td>
<td>72.64(1)</td>
<td></td>
</tr>
<tr>
<td>Gold</td>
<td>Au</td>
<td>79</td>
<td>196.96655(2)</td>
<td></td>
</tr>
<tr>
<td>Hafnium</td>
<td>Hf</td>
<td>72</td>
<td>178.49(1)</td>
<td></td>
</tr>
<tr>
<td>Hassium</td>
<td>Hs</td>
<td>108</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Helium</td>
<td>He</td>
<td>2</td>
<td>4.002602(2)</td>
<td>g, m</td>
</tr>
<tr>
<td>Holmium</td>
<td>Ho</td>
<td>67</td>
<td>164.93032(2)</td>
<td></td>
</tr>
<tr>
<td>Hydrogen</td>
<td>H</td>
<td>1</td>
<td>1.00794(7)</td>
<td>g, m, r</td>
</tr>
<tr>
<td>Indium</td>
<td>In</td>
<td>49</td>
<td>114.818(3)</td>
<td></td>
</tr>
<tr>
<td>Iodine</td>
<td>I</td>
<td>53</td>
<td>126.90447(3)</td>
<td></td>
</tr>
<tr>
<td>Iridium</td>
<td>Ir</td>
<td>77</td>
<td>192.217(3)</td>
<td></td>
</tr>
<tr>
<td>Iron</td>
<td>Fe</td>
<td>26</td>
<td>55.845(2)</td>
<td></td>
</tr>
<tr>
<td>Krypton</td>
<td>Kr</td>
<td>36</td>
<td>83.798(2)</td>
<td>g, m</td>
</tr>
<tr>
<td>Lanthanum</td>
<td>La</td>
<td>57</td>
<td>138.9055(2)</td>
<td>g</td>
</tr>
</tbody>
</table>

Table 13-1. Atomic Weights of the Elements 2001

Continued on next page
Table 13-1. Atomic Weights of the Elements 2001—Continued

<table>
<thead>
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</thead>
<tbody>
<tr>
<td>Terbium</td>
<td>Tb</td>
<td>65</td>
<td>158.92534(2)</td>
<td></td>
<td>Ununquadium</td>
<td>Uuq</td>
<td>114</td>
<td>*</td>
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<td>Thallium</td>
<td>Tl</td>
<td>81</td>
<td>204.3833(2)</td>
<td></td>
<td>Unununium</td>
<td>Uuu</td>
<td>111</td>
<td>*</td>
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</tr>
<tr>
<td>Thorium</td>
<td>Th</td>
<td>90</td>
<td>232.0381(1)*</td>
<td>*g</td>
<td>Uranium</td>
<td>U</td>
<td>92</td>
<td>238.02891(3)*</td>
<td>*g,m</td>
<td>Thulium</td>
<td>Tm</td>
<td>69</td>
<td>168.93421(2)</td>
<td></td>
<td>Vanadium</td>
<td>V</td>
<td>23</td>
<td>50.9415(1)</td>
<td></td>
<td></td>
<td></td>
<td></td>
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<td></td>
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<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Tin</td>
<td>Sn</td>
<td>50</td>
<td>118.710(7)</td>
<td>*g</td>
<td>Xenon</td>
<td>Xe</td>
<td>54</td>
<td>131.293(6)</td>
<td>*g,m</td>
<td>Titanium</td>
<td>Ti</td>
<td>22</td>
<td>47.867(1)</td>
<td></td>
<td>Ytterbium</td>
<td>Yb</td>
<td>70</td>
<td>173.04(3)</td>
<td>*g</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tungsten</td>
<td>W</td>
<td>74</td>
<td>183.84(1)</td>
<td></td>
<td>Yttrium</td>
<td>Y</td>
<td>39</td>
<td>88.90585(2)</td>
<td></td>
<td>Ununbium</td>
<td>Uub</td>
<td>112</td>
<td>*</td>
<td></td>
<td>Zinc</td>
<td>Zn</td>
<td>30</td>
<td>65.409(4)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ununhexium</td>
<td>Uuh</td>
<td>116</td>
<td>*</td>
<td></td>
<td>Zirconium</td>
<td>Zr</td>
<td>40</td>
<td>91.224(2)</td>
<td>*g</td>
<td>Ununnium</td>
<td>Uun</td>
<td>110</td>
<td>*</td>
<td></td>
<td></td>
<td></td>
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</tr>
</tbody>
</table>

Notes: Scaled to the relative atomic mass, $A_r(12\text{C}) = 12$, where $^{12}\text{C}$ is a neutral atom in its nuclear and electronic ground state.

The atomic weights of many elements are not invariant but depend on the origin and treatment of the material. The standard values of $A_r(E)$ and the uncertainties (in parentheses following the last significant figure to which they are attributed) apply to elements of natural terrestrial origin. The footnotes to this table elaborate the types of variation that may occur for individual elements and that may be larger than the listed uncertainties of values of $A_r(E)$. Names of elements with atomic numbers 110 to 116 are provisional.

*Element has no stable nuclides. However, three such elements (Pa, Th, and U) do have a characteristic terrestrial isotopic composition, and for these an atomic weight is tabulated.

†Commercially available Li materials have atomic weights that range between 6.939 and 6.996; if a more accurate value is required, it must be determined for the specific material.

g Geological specimens are known in which the element has an isotopic composition outside the limits for normal material. The difference between the atomic weight of the element in such specimens and that given in the table may exceed the stated uncertainty.

m Modified isotopic compositions may be found in commercially available material because it has been subjected to an undisclosed or inadvertent isotopic fractionation. Substantial deviations in atomic weight of the element from that given in the table can occur.

r Range in isotopic composition of normal terrestrial material prevents a more precise $A_r(E)$ being given; the tabulated $A_r(E)$ value should be applicable to any normal material.

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➤ Write the names of chemical compounds in roman type and treat them as common nouns. (Names for chemical compounds are discussed further in Chapter 12.)

- benzenaldehyde
- calcium carbonate
- chlorobenzene
- ethanol
- hydrochloric acid
- iron(III) nitrate
- isopropyl iodide
- magnesium sulfate
- mercuric sulfate
- methyl salicylate
- phenol
- sodium hydroxide

➤ Use roman type for the symbols for chemical compounds.

\[
\begin{align*}
\text{BaSO}_4 & \quad \text{CH}_3\text{COOH} & \quad \text{NaOH} \\
\text{C}_2\text{H}_5\text{OH} & \quad \text{Fe(NO}_3)_3 & \quad \text{Ni}_3\text{P}_2\text{O}_8 \\
\text{C}_6\text{H}_5\text{Cl} & \quad \text{H}_3\text{PO}_4 & \quad \text{P}_2\text{S}_5 \\
\text{C}_6\text{H}_5\text{OH} & \quad \text{HCl} & \quad \text{VF}_5 \\
\text{CaCO}_3 & \quad \text{HgSO}_4 & \quad \text{Zn(C}_2\text{H}_3\text{O}_2)_2
\end{align*}
\]
You may use both chemical symbols and element names in text, but it is best to use one or the other consistently. Do not mix symbols and words within a name.

NaCl or sodium chloride, not Na chloride

Unnamed elements may be designated by using the atomic number (for example, element 125). They may also be designated by using the systematic name or symbol devised by IUPAC for elements of atomic number greater than 100 that have not yet received trivial names. In this system, an element name consists of a series of numerical roots corresponding to the numerals in the atomic number of the element, followed by “ium.” The roots are as follows:

<table>
<thead>
<tr>
<th>Number</th>
<th>Root</th>
<th>Root</th>
<th>Root</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>nil</td>
<td>4</td>
<td>quad</td>
</tr>
<tr>
<td>1</td>
<td>un</td>
<td>5</td>
<td>pent</td>
</tr>
<tr>
<td>2</td>
<td>bi</td>
<td>6</td>
<td>hex</td>
</tr>
<tr>
<td>3</td>
<td>tri</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The symbols consist of the first letters of the numerical roots.

EXAMPLES

<table>
<thead>
<tr>
<th>Element</th>
<th>Unsystematic Name</th>
<th>Systematic Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>146</td>
<td>unquadhexium</td>
<td>Uqh</td>
</tr>
<tr>
<td>187</td>
<td>unoctseptium</td>
<td>Uos</td>
</tr>
<tr>
<td>209</td>
<td>binilenium</td>
<td>Bne</td>
</tr>
<tr>
<td>290</td>
<td>biennilium</td>
<td>Ben</td>
</tr>
<tr>
<td>501</td>
<td>pentnilunium</td>
<td>Pnu</td>
</tr>
<tr>
<td>502</td>
<td>pentnilbium</td>
<td>Pnb</td>
</tr>
<tr>
<td>503</td>
<td>pentniltrium</td>
<td>Pnt</td>
</tr>
<tr>
<td>900</td>
<td>ennilnilium</td>
<td>Enn</td>
</tr>
</tbody>
</table>

Drop the final “n” in “enn” when it is followed by “nil” (see elements 290 and 900) and the final “i” in “bi” and “tri” when they are followed by “ium” (see elements 502 and 503).

You may use common abbreviations for organic groups in formulas and structures, but not in text. These (and only these) abbreviations need not be defined.

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Acetyl</th>
<th>Aryl</th>
<th>Butyl</th>
<th>Isobutyl</th>
<th>Sec-Butyl</th>
<th>Tert-Butyl</th>
<th>Benzoyl</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ac</td>
<td>acetyl</td>
<td>aryl</td>
<td>butyl</td>
<td>isobutyl</td>
<td>sec-butyl</td>
<td>tert-butyl</td>
<td>benzoyl</td>
</tr>
<tr>
<td>Ar</td>
<td>methyl</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Use square brackets in formulas for coordination entities.

\[ \text{[Cr(C}_6\text{H}_6\text{)}_2] \]
\[ \text{K[PtCl}_3\text{(C}_2\text{H}_4\text{)]} \]
In the formula for an *addition compound*, use a centered dot, closed up on each side. (Although the IUPAC books show a space on each side, this spacing would wreak havoc with many typesetting systems.)

\[
\text{BH}_3\cdot\text{NH}_3 \\
\text{Ni(NO}_3\text{)}_2\cdot2\text{Ni(OH)}_2
\]

*Water of hydration* follows a centered dot, closed up on each side.

\[
\text{Na}_2\text{SO}_4\cdot10\text{H}_2\text{O} \\
\text{Zn(NO}_3\text{)}_2\cdot\text{H}_2\text{O}
\]

Use either a slash or an en dash between components of a mixture, but not a colon.

- dissolved in 5:1 glycerin/water
- dissolved in 5:1 glycerin–water
- the metal/ligand (1:1) reaction mixture
- the metal–ligand (1:1) reaction mixture
- the metal–ligand (1/1) reaction mixture
- the methane/oxygen/argon (1/50/450) matrix
- the methane/oxygen/argon (1:50:450) matrix

**Reference to the Periodic Table**

- Always use lowercase for the word “group”, even with a specific number.
  
  - group 15 elements
  - group IVB elements

- Always use lowercase for the words “periodic table”.
  
  - The elements in group 8 of the periodic table include Fe, Ru, and Os.

**Atoms and Molecules**

Nuclide descriptors are specified with superscripts and subscripts to the element symbol, as follows.

**Use the Left Superscript for Mass Number**

- The mass number of an atom is usually shown only for isotopes or in discussions of isotopes.

\[
^{12}\text{C} \\
^{35}\text{Cl} \\
^{32}\text{S}
\]
Use the Left Subscript for Atomic Number

- The atomic number of an atom is usually used only in discussions of nuclear chemistry.

\[ _6\text{C} \quad _{16}\text{S} \]

Use the Right Superscript for Ionic Charge

- The charge number is followed by the sign of the ionic charge. When the charge number is 1, only the sign is used.

\[ \text{Ca}^{2+} \quad \text{Na}^{+} \quad \text{NO}_3^- \]

- Stagger the subscript and superscript; do not align them. The subscript comes first with ionic charge.

\[ \text{PO}_4^{3-} \]

- Do not use multiple plus or minus signs, and do not circle the charge.

\[ \text{Hg}^{2+} \; (\text{not} \; \text{Hg}^{++}) \]

Use the Right Asterisk for Excited Electronic State

- \[ \text{He}^* \quad \text{NO}^* \]

Use the Right Superscript for Oxidation Number

- You may use superscript roman numerals for oxidation numbers. In formulas, do not use numbers on the line to avoid confusion with the symbols for iodine or vanadium.

\[ \text{Co}^{\text{III}} \quad \text{Mn}^{\text{III}}/\text{Mn}^{\text{IV}} \quad \text{O}^{-\text{II}} \]
\[ \text{Fe}^{\text{II}}\text{Cl}_3 \quad \text{Mn}^{\text{IV}}\text{O}_2 \quad \text{Pb}^{\text{IV}}\text{O}_2 \]
\[ \text{Mn}^{\text{III/IV}} \quad (\text{NH}_3)_2\text{Pt}^{\text{II}} \quad \text{Ru}^{\text{II/III}} \]
\[ \text{Mn}^{\text{III}}-\text{Mn}^{\text{IV}} \quad \text{Ni}^{\text{0}} \quad \text{Ru}^{\text{II}}/\text{Ru}^{\text{III}} \]

- Stagger the subscript and superscript; do not align them. The subscript follows the superscript with oxidation number.

\[ \text{Pb}^{\text{II}}_2 \]

- You may also write oxidation numbers on the line in parentheses closed up to the element name or symbol.
cobalt(III) or Co(III)
copper(II) or Cu(II)
diammineplatinum(II)
ferrate(VI) ion
iron(II) or Fe(II)
iron(II) chloride
manganese(IV) oxide
Mn(III)–Mn(IV) complex
Mn(III)/Mn(IV) complex
potassium tetracyanonickelate(0)

Use the Right Subscript for Number of Atoms

➤ With an element symbol, use a subscript to indicate the number of atoms, whether in formulas or in narrative text.

\[
\begin{align*}
\text{Al}_2\text{O}_3 & \quad \text{(CH}_3 \text{)_4C} & \quad \text{H}_2\text{S} \\
\text{C}_6 & \quad \text{Fe}_3 & \quad \text{NH}_4 \\
\text{C}_6\text{H}_5\text{CH}_3 & \quad \text{FeSi}_2
\end{align*}
\]

The C\text{60} fullerene molecule is shaped like a soccer ball.

➤ With an element name, follow the usual conventions for numbers in text.

Molecules composed of 60 carbon atoms are shaped like soccer balls.

In this reaction, three hydrogen atoms are lost.

Atom in a Specific Position

➤ Use either words or symbols and numbers on the line to refer to an atom in a specific position.

at the carbon in the 6-position or at C6 or at C-6

the atom in the β-position or the β atom

Isotopes

➤ Specify the isotope of an element by a mass number written as a left superscript to the element symbol.

\[
\begin{align*}
^{13}\text{C} & \\
^{15}\text{N} & \\
^{32}\text{S} & \\
^{29}\text{Si} & \\
^{235}\text{U}
\end{align*}
\]
Alternatively, indicate an isotope by using the spelled-out element name hyphenated to its mass number.

- carbon-14
- uranium-235

In either case, the isotope name or symbol is pronounced first, then the number. Thus, $^{14}$C is pronounced “c fourteen”. Consequently, choose the article (a or an) preceding the isotope to accommodate the pronunciation of the element name or symbol, not the number.

- a carbon-14 isotope: a $^{14}$C (pronounced “c fourteen”)
- a hydrogen-3 isotope: an $^{3}$H (pronounced “aitch three”)
- a nitrogen-15 isotope: an $^{15}$N (pronounced “en fifteen”)

Use the symbols $^2$H or D for deuterium and $^3$H or T for tritium when no other nuclides are present.

- $^2$H or D
- $^3$H or T

An *isotopically unmodified* compound is one whose isotopic nuclides are present in the proportions that occur in nature. An *isotopically modified* compound has a nuclide composition that deviates measurably from that occurring in nature.

An *isotopically substituted* compound has a composition such that all of the molecules of the compound have only the indicated nuclides at the designated positions. To indicate isotopic substitution in formulas, the nuclide symbols are incorporated into the formulas. To indicate isotopic substitution in spelled-out compound names, the number and symbol (and locants if needed) are placed in parentheses closed up to the name.

<table>
<thead>
<tr>
<th>Isotopically Unmodified</th>
<th>Isotopically Modified</th>
<th>Isotopically Substituted</th>
</tr>
</thead>
<tbody>
<tr>
<td>H$_2$N$^{14}$CONH$_2$</td>
<td>CH$_3$O$^{3}$H</td>
<td>H$_2$N$^{15}$F$_2$</td>
</tr>
<tr>
<td>$^{23}$NaCl</td>
<td>(T$_2$N)$_2$CO</td>
<td>$^{2}$H$_2$S</td>
</tr>
<tr>
<td>$^{14}$CH$_4$</td>
<td>CH$_2$THO</td>
<td>$^{2}$H$_2$SO$_4$</td>
</tr>
<tr>
<td>$^{24}$NaCl</td>
<td>Na$_2$$^{35}$S</td>
<td>$^{3}$H$_2$</td>
</tr>
<tr>
<td>$^{23}$NaCl</td>
<td>$^{32}$PO$_4^{3-}$</td>
<td>$^{18}$O$^{2}$H</td>
</tr>
<tr>
<td>$^{14}$CH$_4$</td>
<td>Mo($^{12}$CO)$_6$</td>
<td>$^{(15}$N)ammonia</td>
</tr>
<tr>
<td>$^{23}$NaCl</td>
<td>$^{23}$UCl$_3$</td>
<td>($^{14}$C$_6$)glucose</td>
</tr>
<tr>
<td>$^{14}$CH$_4$</td>
<td>H$_2$N$^{15}$F$_2$</td>
<td>(1,3-$^3$H$_2$)benzene</td>
</tr>
<tr>
<td>$^{14}$CH$_4$</td>
<td>$^{14}$CH$_4$</td>
<td>1-chloro(2-$^3$H)benzene</td>
</tr>
</tbody>
</table>

An *isotopically labeled* compound is a mixture of an isotopically unmodified compound with an analogous isotopically substituted compound or compounds. Isotopically labeled compounds may be specifically labeled or selectively labeled. To indicate isotopic labeling, the number and symbol (and locants if needed) are enclosed in square brackets closed up to the compound name or formula.

**Specifically Labeled:**

- [$^{14}$C]H$_4$
- CH$_2$[$^3$H$_2$]
- CH$_3$CH$_2$[$^{18}$O]H
SELECTIVELY LABELED:

\[ ^2\text{H}\text{CH}_4 \]
\[ ^2\text{H}\text{PH}_3 \]
\[ ^{36}\text{Cl}\text{SOCl}_2 \]
\[ [6,7-^{15}\text{N}]\text{adenosine} \]
\[ [^{15}\text{N}]\text{alanine} \]
\[ [^{15}\text{N}]\text{ammonium chloride} \]
\[ [1,3-^3\text{H}_2]\text{benzene} \]
\[ [^{57}\text{Co}]\text{cyanocobalamin} \]
\[ 2,4\text{-diamino}[^{18}\text{O}]\text{phenol} \]
\[ [2,8-^3\text{H}]\text{inosine} \]
\[ [2-^{14}\text{C}]\text{leucine} \]

➤ When the isotope position is specified by a group name that is part of the parent compound, italicize the group name.

\[ [\text{methyl}^{14}\text{C}]\text{toluene} \]

➤ Isotopically labeled compounds may also be described by inserting the symbol in brackets into the name of the compound.

- hydrogen \[ ^{36}\text{Cl}\text{chloride} \]
- \[ ^{35}\text{S}\text{sulfuric} [^{2}\text{H}]\text{acid} \]

➤ Do not use the left superscript within an abbreviation.

\[ [^{32}\text{P}]\text{CMP (not CM}^{32}\text{P)} \]

➤ To indicate general labeling, use the symbol G in the names of selectively labeled compounds in which all positions of the designated element are labeled, but not necessarily in the same isotopic ratio.

\[ d-[G-^{14}\text{C}]\text{glucose} \]

➤ To indicate uniform labeling, use the symbol U in the names of selectively labeled compounds in which all positions of the designated element are labeled in the same isotopic ratio.

\[ d-[U-^{14}\text{C}]\text{glucose} \]

➤ When it is unknown or irrelevant whether the compound is isotopically labeled or isotopically substituted, simply hyphenate the isotope symbol to the compound name and do not use square brackets or parentheses.

\[ ^{14}\text{C}-\text{glucose} \]
\[ ^3\text{H}-\text{benzene} \]
\[ ^{15}\text{N}-\text{adenosine} \]

The Boughton system, used in Chemical Abstracts, does not distinguish between labeling and substitution. The isotopic variation is shown by the symbol for the isotope (with a subscript numeral to indicate the number of isotopic atoms) placed after the name or relevant portion of the name; locants are cited
if necessary. The locants and symbols are in italics, except subscripts and Greek letters, and hyphens are used to separate them.

acetamide-\textit{1-}^{13}\textit{C}^{15}\textit{N}
acetic-\textit{17}\textit{O}_2\textit{ acid}
benzeneacetic-\textit{carboxy}\textit{,}\textit{\alpha}^{-14}\textit{C}_2\textit{ acid}
benzoic-\textit{18}\textit{O} acid
4-(2-propenyl-3-\textit{13}\textit{C}-oxy)benzoic acid
toluene-\textit{methyl}^{-14}\textit{C}

In this system, deuterium and tritium are represented by italic lowercase letters \(d\) and \(t\), respectively.

acetic-\(t_t\) acid-\(t\)
alanine-\(N,N,1-d_3\)
ammonia-\(d-t\)
ethane-\(1-d-2-t\)
1-(ethyl-\(2,2,2-d_3\))-4-(methyl-\(d_3\))benzene
methan-\(t\)-ol
methane-\(d_4\)
tri(silyl-\(d_3\))phosphine
urea-\(t_q\)

Radicals

In the formula of a free radical, indicate the unshared electron by a superscript or centered dot closed up to the element symbol or formula. The superscript dot comes after the symbol or formula; centered dots come before or after the symbol or formula.

\[
\begin{array}{ccc}
\text{Br}^- & \text{H}^- & \cdot\text{SH} \\
\text{Br}^+ & \text{HO}^- & (\text{SiH}_3)^+ \\
\cdot\text{CH}_3 & \cdot\text{NH}_2 & \cdot\text{SnH}_3 \\
\text{C}_6\text{H}_5^- & & \\
\end{array}
\]

Charged radical cations and anions are often indicated by the symbol, formula, or structure with a superscript dot followed by a plus or minus sign. However, in mass spectrometry, the reverse is used. Therefore, use the order of dots and signs for charges that is appropriate for the context.

\[
\begin{array}{ccc}
\text{(Ag}_2\text{)}^+ & \text{R}^- & \text{R}^{+}(2-) \\
\text{C}_6\text{H}_5\text{NO}^- & \text{R}_2^{+} & (\text{SO}_2)^{--} \\
\text{HCO}^+ & & \\
\end{array}
\]

MASS SPECTROMETRY

\[
\begin{array}{ccc}
\text{C}_2\text{H}_6^{+} & \text{R}^{+} & \\
\end{array}
\]
**Bonds**

➤ For linear formulas in text, do not show single bonds unless the bonds are the subject of the discussion.

\[
\begin{align*}
C_6H_5CH_3 \\
C_6H_5COOCOCH_3 \\
CH_3CHOHCH_3 \\
CH_3COOH \\
H_2SO_4
\end{align*}
\]

➤ When necessary for the discussion, indicate bonds by en dashes.

- the \(-\text{CH}_2-\) segment
- the C–H distances
- the C–C–C angle
- \((-\text{CH}_2-\text{CH}(\text{CH}_3)-\text{O}-)_n\)

➤ When necessary, show double and triple bonds in linear formulas.

\[
\begin{align*}
\text{CH}_3\text{C}=\text{CH} \\
\text{CH}_2=\text{CH}_2 \\
\text{R–C–OH} & \text{ is better as } \text{RCOOH or } \text{RCO}_2\text{H or } \text{RC}(=\text{O})\text{OH} \\
& | \\
& 0
\end{align*}
\]

➤ Use three centered dots to indicate association of an unspecified type (e.g., hydrogen bonding, bond formation, or bond breaking).

\[
\begin{align*}
\text{C⋯Pt} \\
\text{F⋯H–NH}_3 \\
\text{H}_2\text{O⋯π aromatic hydrogen bonding} \\
\text{Mg}^{2+}\cdots\text{O–} \\
\text{Ni⋯Al}
\end{align*}
\]

**Crystallography**

**Planes and Directions in Crystals**

➤ Miller indices of a crystal face or a single net plane are enclosed in parentheses. \((123)\) or \((hkl)\) is a plane or set of planes that describe crystal faces; \((h_1h_2h_3)\) is a single net plane.

➤ Laue indices are not enclosed. 123 or \(hkl\) is the Bragg reflection from the set of net planes \((123)\) or \((hkl)\), respectively.
Indices of a set of all symmetrically equivalent crystal faces or net planes are enclosed in braces. \{hkl\} is a form.

Indices of a zone axis or lattice direction are enclosed in square brackets. [123] or [uvw] is a direction.

Indices of a set of symmetrically equivalent lattice directions are enclosed in angle brackets. \langleuvw\rangle represents all crystallographically equivalent directions of the type [uvw].

\begin{align*}
120 \\
1,10,1 \\
11,0,1 \\
1,–2,0 reflections \\
the (111) face \\
the (120) face \\
the [001] axis \\
the [010] direction \\
the [101] direction \\
h00 diffraction lines \\
the hk0 zone \\
the 002 reflection \\
the 00l class of reflections
\end{align*}

When indices are used with spelled-out element names, separate the name of the element and the index with a space.

- copper (111)
- rhenium (010)
- a gold (111) substrate
- on silicon (111) surfaces
- the silver (110) surface

However, when indices are used with element symbols, close up the element symbol to the index.

- Au(210)
- CdTe(100)
- Cu(111)
- GaAs(100)
- Rh(010)
- Si(400)

- an iodine-modified Ag(111) electrode
- the Ag(110) surface
Types of Crystal Lattices

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>bcc</td>
<td>body-centered cubic</td>
</tr>
<tr>
<td>ccp</td>
<td>cubic close-packed</td>
</tr>
<tr>
<td>fcc</td>
<td>face-centered cubic</td>
</tr>
<tr>
<td>hcp</td>
<td>hexagonal close-packed</td>
</tr>
</tbody>
</table>

Symmetry Operations and Structural Point Groups

➤ Use italic type for the letters in symmetry operations and structural point groups. The symbols (Schoenflies) are as follows: \(E\), identity; \(C\), cyclic; \(D\), dihedral; \(T\), tetrahedral; \(O\), octahedral; \(I\), icosahedral; \(S\), rotation–reflection; and \(\sigma\), mirror plane. Align subscripts and superscripts.

\[
\begin{align*}
C_1 & \quad C_{2h} & \quad S_3 \\
C_i & \quad C_{3h} & \quad S_4 \\
C_s & \quad D_{2d} (V_d) & \quad 2S_6 \\
C_2 & \quad D_{3d} & \quad S_8 \\
C_3 & \quad D_{4d} & \quad \sigma \\
C_4 & \quad D_{2h} (V_h) & \quad 2\sigma_v \\
C_{\infty c} & \quad D_{3h} & \quad 3\sigma_v \\
C_{2v} & \quad D_{4h} & \quad 4\sigma_v \\
C_{3v} & \quad D_{\infty h} & \quad 3\sigma_d \\
C_{\infty v} & \quad I_h & \quad \sigma_h \\
C_{\infty v} & \quad O_h (K_h) & \quad T_d
\end{align*}
\]

Crystallographic Point Groups

➤ Use arabic numerals or combinations of numerals and the italic letter \(m\) to designate the 32 crystallographic point groups (Hermann–Mauguin). The number is the degree of the rotation, and \(m\) stands for mirror plane. Use an overbar to indicate rotation inversion.

<table>
<thead>
<tr>
<th>Number</th>
<th>Symbol</th>
<th>Space Group</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>km</td>
<td>6/mkm</td>
</tr>
<tr>
<td>(m)</td>
<td>4mm</td>
<td>4(\bar{m})</td>
</tr>
<tr>
<td>(2/m)</td>
<td>32</td>
<td>(m\bar{3}m)</td>
</tr>
<tr>
<td>(mm2)</td>
<td>622</td>
<td></td>
</tr>
</tbody>
</table>

Space Groups

➤ Designate space groups by a combination of unit cell type and point group symbol, modified to include screw axes and glide planes (Hermann–Mauguin); 230 space groups are possible. Use italic type for conventional types of unit cells (or Bravais lattices): \(P\), primitive; \(I\), body-centered; \(A\), A-face-centered; \(B\), B-face-centered; \(C\), C-face-centered; \(F\), all faces centered; and \(R\), rhombohedral.
Crystallographic Information File

A description of the Crystallographic Information File, CIF, is included in Appendix 13-2.

Chirality

➤ Use italic type for certain chirality symbols and symmetry site terms.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>anticlockwise</td>
<td>OC</td>
<td>octahedron</td>
</tr>
<tr>
<td>C</td>
<td>clockwise</td>
<td>TP</td>
<td>trigonal phase</td>
</tr>
<tr>
<td>CU</td>
<td>cube</td>
<td>TPR</td>
<td>trigonal prism</td>
</tr>
<tr>
<td>DD</td>
<td>dodecahedron</td>
<td>TPY</td>
<td>trigonal pyramid</td>
</tr>
</tbody>
</table>

These symbols are often combined with coordination numbers and position designations for stereochemical descriptors (e.g., OC-6-11').

➤ In chemical names, use (R) and (S), with designated locants when applicable, as prefixes to designate absolute configuration.

- (R)-hydroxyphenylacetic acid
- (S)-2,3-dihydroxypropanoic acid
- (1S,2S,4R)-trichloro-1,2,4-trimethylcyclohexane

➤ Indicate optical rotation by plus and minus signs in parentheses and hyphenate them to the chemical name.

- (±)-4-(2-aminopropyl)phenol
- (+)-glucose
- (–)-tartaric acid

➤ Use small capital letters D and L for absolute configuration with amino acids and carbohydrates.

- β-D-cellotetraose
- d-allothreonine
- d-glucose
- d-valine
- DL-leucine
- hydroxy-DL-glutamic acid
- 5-hydroxy-L-lysine
- hydroxy-L-proline
- L-alanine
- L-alloisoleucine
- L-ascorbic acid
- L-phenylalanine
➤ Use a hyphen between (+) or (−) and d or l.

(−)-d-fructose
(−)-d-glyceraldehyde
(+)-l-phosphoglycerol

Concentration

➤ Use square brackets enclosing an element symbol or formula to indicate its concentration in reactions and equations, but not in narrative text.

**Correct**

\[\text{[Mg}^{2+}\text{]} = 3 \times 10^{-2} \text{ M}\]

The Mg concentration decreased with repeated washings.

**Incorrect**

The \([\text{Mg}]\) was found to be greater in the unwashed samples.

➤ Do not use square brackets to indicate concentration with a spelled-out name.

\[[\text{Ca}^{2+}] \ (\text{not \ [calcium]\})\]

\[[\text{NaCl}] \ (\text{not \ [sodium chloridr]}\)]

➤ Do not use italic type for the chemical concentration unit M (molar, moles per cubic decimeter, moles per liter) or the unit N (normal). Use italic type for the unit \(m\) (molal, moles per kilogram). Use a space between the number and these abbreviations, that is, on each side of these abbreviations.

- 8 M urea
- 1 mM EDTA
- 6 N HCl
- 2.0 \(m\) NaOH

➤ When concentration is given as percentage, use the percent sign closed up to the number.

- 20% \(H_2SO_4\)
- 90% acetonitrile/10% water

➤ Generally, the negative logarithm of the hydrogen ion concentration is denoted by \(pH\); the negative logarithm of the hydroxide ion concentration is denoted by \(pOH\). Use a space to separate \(pH\) or \(pOH\) and the number. Use
roman type for pH and pOH; always use lowercase for “p”; always capitalize “H” and “OH”.

Solutions were titrated to pH >11.
The UV spectra were measured at pH 6.
A pOH of <12 was acceptable.

### Chemical Reactions

➤ Short chemical reactions may be run into text or they may be displayed and numbered, if numbering is needed. Long chemical reactions should be displayed separately from the text. The sequential numbering system used may integrate both chemical and mathematical equations, or separate sequences using different notations may be used for different types of equations (e.g., eqs 1–3 could be used for a set of chemical reactions and eqs I–III could be used for a set of mathematical equations). The use of lettering, rather than numbering, sequences is also acceptable.

\[
\text{Cr(CO)}_4 + \text{CO} \rightarrow \text{Cr(CO)}_5 \quad (1)
\]

\[
\text{NH}_3 + \text{HCOOH} \rightarrow \text{NH}_2\text{CHO} + \text{H}_2\text{O} \quad (2)
\]

\[
(C_6\text{H}_5)_2\text{P} - \text{P}(C_6\text{H}_5)_2 \rightarrow 2(C_6\text{H}_5)_2\text{P} \quad (3)
\]

\[
\text{Fe(CO)}_5 + \text{OCH}_2^- \rightarrow \text{Fe(CO)}_4(\text{CO}_2\text{CH}_3)^- \quad (4)
\]

➤ Many kinds and combinations of arrows can be used. For example, two full arrows in opposite directions (⇌) indicate a reaction that is proceeding in both directions. Two arrows with half heads in opposite directions (⇌) indicate a reaction in equilibrium. A single arrow with heads on both sides (⇋) indicates resonance structures, not a reaction.

➤ Specify the number of each species (molecules, atoms, ions, etc.) of reactants and products by a numeral written on the line and closed up to the symbol.

\[
2\text{Al} + 6\text{NaOH} \rightarrow 2\text{Na}_3\text{AlO}_3 + 3\text{H}_2 \quad (5)
\]

➤ To indicate the aqueous, solid, liquid, or gas state, use the appropriate abbreviations on the line, in parentheses, and with no space preceding them.

\[
\text{Ag(s)} + \text{H}^+(\text{aq}) + \text{Cl}^-(\text{aq}) \rightarrow \text{AgCl(s)} + \frac{1}{2}\text{H}_2(\text{g}) \quad (6)
\]

\[
4\text{FeS(s)} + 7\text{O}_2(\text{g}) \rightarrow 2\text{Fe}_2\text{O}_3(\text{s}) + 4\text{SO}_2(\text{g}) \quad (7)
\]

➤ Indicate reaction conditions and catalysts over and under the arrow in a smaller type size. The Greek capital letter delta indicates heat; h\nu indicates light, where h is Planck’s constant and the Greek letter nu is the photon frequency.
Chapter 13: Conventions in Chemistry ➤ 273

\[
\text{PhS}^- \xrightarrow{hv} \text{PhS}^+ + e^- \\
\text{C}_3\text{H}_8(g) + 5\text{O}_2(g) \xrightarrow{\Delta} 3\text{CO}_2(g) + 4\text{H}_2\text{O}(g) \\
\text{RC≡N} + 2\text{H}_2 \xrightarrow{\text{Pt or Pd}} \text{RCH}_2\text{NH}_2 \\
2\text{H}_2\text{O} + \text{CH}_3\text{C(=O)}\text{CH}_3 \xrightarrow{\text{KMnO}_4, \text{H}_2\text{SO}_4, \Delta} 2\text{CH}_3\text{C}(=\text{O})\text{CH}_3 + 2\text{H}_2 \\
(\text{C}_2\text{H}_5)_2\text{C}=\text{O} + 2\text{CH}_3\text{OH} \xrightarrow{\text{H}^+ \text{at } 125^\circ\text{C}} (\text{C}_2\text{H}_5)_2\text{C(OCH}_3)_2 + \text{H}_2\text{O}
\]

➤ Specify nuclear reactions according to the following scheme:

\[
\begin{array}{c}
\text{initial nuclide} \\
\text{incoming particle(s), or quanta} \\
\text{outgoing particle(s), or quanta} \\
\text{final nuclide}
\end{array}
\]

**EXAMPLES**

\[
^{14}\text{N}(\alpha,\text{p})^{17}\text{O} \\
^{59}\text{Co}(\text{n},\gamma)^{60}\text{Co} \\
^{23}\text{Na}(\gamma,3\text{n})^{20}\text{Na} \\
^{31}\text{P}(\gamma,\text{pn})^{29}\text{Si}
\]

➤ Treat chemical equations that include structures with rings as illustrations. They are discussed in Chapter 17.

➤ Abbreviate reaction types with capital roman letters and arabic numerals.

\[
\begin{array}{cc}
\text{S}_\text{N}1 & \text{S}_\text{N}2 \\
\text{E1} & \text{E2} \\
\text{S}_\text{RN}1 & \text{S}_\text{RN}2
\end{array}
\]

first- and second-order nucleophilic substitution, respectively

first- and second-order elimination, respectively

first- and second-order radical nucleophilic substitution, respectively

➤ Subscripts denote a chemical process or reaction.

\[
\begin{array}{c}
\text{ads} \\
\text{at} \\
\text{c} \\
\text{dil} \\
\text{dpl} \\
\text{f} \\
\text{fus} \\
\text{imm} \\
\text{mix} \\
\text{r} \\
\text{sol} \\
\text{sub} \\
\text{trs} \\
\text{vap}
\end{array}
\]

adsorption
atomization
combustion
dilution
placement
formation
fusion
immersion
mixing
reaction in general
solution
sublimation
transition
vaporization
Certain superscripts are recommended.

- ‡ activated complex, transition state
- ′ apparent
- E excess quantity
- id ideal
- ∞ infinite dilution
- * pure substance
- °, ‖ standard state

Reporting Analytical Data

There is no best way to present data. A presentation that is suitable for one paper or publication may be unsuitable for another. The following are examples of acceptable presentations of analytical data. These are not necessarily real examples; they may be combinations of data from two or more samples, intended to show various style possibilities. You need not define the abbreviations and symbols in the paper.

Melting and Boiling Points

mp 175.5 °C (lit.\(^25\) mp 175–176 °C)
mp 225 °C dec
bp 127 °C

Abbreviations: mp, melting point; bp, boiling point; lit., literature value; and dec, decomposition. A full space is used between the number and the unit °C; the degree symbol is closed up to the C. A superscript number after “lit.” denotes the number of the reference.

Specific Rotation

\([\alpha]_D^{20} + 25.4\) (c 1.00, CHCl\(_3\))

Abbreviations: \(\alpha\), specific rotation; D, the sodium D line or wavelength of light used for the determination; and the superscript number, temperature (°C) at which the determination was made. In parentheses: c stands for concentration; the number following c is the concentration in grams per 100 mL of solution; and last is the solvent name or formula.

NMR Spectroscopy

\(^1\)H NMR (400 MHz, CD\(_3\)OD, δ): 8.73 (s, 3H, –OCH\(_3\)), 7.50 (s, 1H, CH), 7.15 (d, \(J = 8.2\) Hz, 1H, Ar H), 6–3 (br s, 5H, NH and NH\(_2\)).

Compound 5: \(^1\)H NMR (500 MHz, CDCl\(_3\), δ) 1.12 (t, \(J = 7.1\) Hz, –CH\(_2\)CH\(_3\), 3H), 3.34 (q, \(J = 7.1\) Hz, –CH\(_2\)CH\(_3\), 2H), 3.38 (t, \(J = 6.0\) Hz, –CH\(_2\)CH\(_2\)OH, 2H), 3.72 (t, \(J = 6.0\) Hz, –CH\(_2\)CH\(_2\)OH, 2H), 6.57 (dd, \(J = 8.7\) Hz, Ar H, 2H).

\(^{13}\)C NMR (DMSO-\(d_6\), δ): 175.4 (C=O), 156.5 (\(C_4\)), 147.4 (\(C_6\)), 138.3 (\(C_2\)), 110.5 (d, \(J = 11.3\) Hz, \(C_5\)), 52.3 (CH\(_3\)), 28.4 and 28.8 (\(C_7\)).
$^{13}$C NMR (DMSO-$d_6$, $\delta$): 0.43 (2C), 27.56 (4C), 131.8 (1C), 161.9 (2C).

$^{13}$C NMR (CDCl$_3$, 75.4 MHz): $\delta$ 213.50 (s, C-21), 178.27 (s, C-2), 168.69 (s, C-8), 164.61 (d, C-10), 119.67 (d, C-7), 52.45 (t, C-22), 38.95 (q, C-25).

$^{13}$C NMR ($C_6D_{12}$, $\delta$): 6.51 (s, C$_5$Me$_5$), 14.41 (d, $J$ = 157 Hz, PMe$_3$), 28.68 (s, Me), 105.1 (t, $J$ = 3.7 Hz, C$_5$Me$_3$), 128.52 (s), 135.19 (br s), 212.56 (C=O).

If the experimental conditions have already been described elsewhere in the paper, they need not be repeated.

NMR: 3.81, 2.56, and 2.12 ppm.

Compound 27: NMR 5.14, 3.90, 2.67, and 1.88 ppm.

Abbreviations: $\delta$, chemical shift in parts per million (ppm) downfield from the standard; $J$, coupling constant in hertz; and the multiplicities s, singlet; d, doublet; t, triplet; q, quartet; and br, broadened. Italicized elements or groups are those that are responsible for the shifts.

**IR Spectroscopy**

IR (KBr) $\bar{\nu}$$_{\text{max}}$: 967 (Ti=O), 3270 cm$^{-1}$ (NH).

IR (KBr, thin film) $\bar{\nu}$$_{\text{max}}$ (cm$^{-1}$): 3017, 2953 (s, OH), 2855 (s), 2192, 1512, 1360, 1082, 887.

IR (dry film) $\bar{\nu}$$_{\text{max}}$: 3324 (OH), 2973–2872 (CH, aliphatic), 1706 (C=O, ketone), 1595, 1437, 1289, 1184, 1048, 870, 756, 677 cm$^{-1}$.

IR: 2000, 2030, 2040, 2050 cm$^{-1}$.

IR (cm$^{-1}$): 3130, 3066, 2964, 1654, 1500, 1371.

Compound 6: IR 2910, 2487, 1972, 1564, 1190 cm$^{-1}$.

Abbreviations: $\bar{\nu}$$_{\text{max}}$ is the wavenumber of maximum absorption peaks in reciprocal centimeters, and the absorptions are w, weak; m, medium; s, strong; vw, very weak; vs, very strong; and br, broad.

**Mass Spectrometry**

MS $m/z$ (relative intensity): 238.2058 (44.8%), 195.1487 (100%), 153.1034 (21.2%).

GC–MS $m/z$ (% relative intensity, ion): 202 (9, M + 4), 200 (32, M + 2), 198 (23, M$^+$), 142 (35, M − 2CO), 321 (95, M − Me), 415 (M$^+$ − Cl).

HRMS–FAB ($m/z$): [M + H]$^+$ calcd for C$_{21}$H$_{38}$N$_4$O$_6$S, 475.259; found, 475.256.

EIMS (70 eV) $m/z$: M$^+$ 420 (15), 241 (15), 201 (59), 135 (14), 69 (23).

Abbreviations: $m/z$ is the mass-to-charge ratio, M is the molecular weight of the molecule itself, M$^+$ is the molecular ion, HRMS is high-resolution mass spectrometry, FAB is fast atom bombardment, and EIMS is electron-impact mass spectrometry.
UV–Visible Spectroscopy

UV (hexanes) $\lambda_{\text{max}}$, nm ($\varepsilon$): 250 (1070).

UV (CH$_3$OH) $\lambda_{\text{max}}$ (log $\varepsilon$) 210 (3.33), 242 (sh, 3.02), 288 (sh, 2.21), 421 nm (3.16).

Abbreviations: $\lambda_{\text{max}}$ is the wavelength of maximum absorption in nanometers; $\varepsilon$ is the molar absorption coefficient or molar absorptivity; and sh is the shoulder. The wavenumber, $\tilde{\nu}$, in reciprocal micrometers, might also be given.

Quantitative Analysis

Anal. Calcd for C$_{45}$H$_{28}$N$_4$O$_7$: C, 62.47; H, 3.41; N, 6.78. Found: C, 61.80; H, 3.55; N, 6.56.

All values are given as percentages.

X-ray Diffraction Spectroscopy

Separate the element and its spectral line by a space.

- Au L$_1$
- Au L$_{III}$
- Cr K
- Cu K$\alpha$
- Cu K$\beta$
- Mo K$\alpha$

Citing ASTM, ANSI, and ISO Standards

ASTM International, originally known as the American Society for Testing and Materials; ANSI, the American National Standards Institute; and ISO, the International Organization for Standardization, are organizations that set standards in a variety of areas.

For ASTM standards, separate the letter and the number of the standard by a space. For ANSI standards, close up the letter and the number.

ASTM

- D 3137
- D 573
- D 130
- D 1660
- as described in ASTM Standard D 1223

ANSI

- Z358.1-1990
- Z88.2-1992
- as noted in ANSI Standard H35.1M-1993

ISO

- 14020
- 9000
- 71.040
- ISO/DIS 14010
- according to ISO Standard 11634
## APPENDIX 13-1

### Symbols for Commonly Used Physical Quantities

#### Atoms and Molecules

<table>
<thead>
<tr>
<th>Name</th>
<th>Symbol</th>
<th>SI Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Atomic mass</td>
<td>( m_a )</td>
<td>kg</td>
</tr>
<tr>
<td>Atomic mass constant</td>
<td>( m_u )</td>
<td>kg</td>
</tr>
<tr>
<td>Atomic number</td>
<td>( Z )</td>
<td>dimensionless</td>
</tr>
<tr>
<td>Decay constant</td>
<td>( \lambda )</td>
<td>s(^{-1})</td>
</tr>
<tr>
<td>Electron rest mass</td>
<td>( m_e )</td>
<td>kg</td>
</tr>
<tr>
<td>Electronic term</td>
<td>( T_e )</td>
<td>m(^{-1})</td>
</tr>
<tr>
<td>Elementary charge (of a proton)</td>
<td>( e )</td>
<td>C</td>
</tr>
<tr>
<td>g factor, g value</td>
<td>( g )</td>
<td>dimensionless</td>
</tr>
<tr>
<td>Ionization energy</td>
<td>( E_p )</td>
<td>J</td>
</tr>
<tr>
<td>Magnetogyric ratio</td>
<td>( \gamma )</td>
<td>s(^{-1})·T(^{-1})</td>
</tr>
<tr>
<td>Mass number</td>
<td>( A )</td>
<td>dimensionless</td>
</tr>
<tr>
<td>Neutron number</td>
<td>( N )</td>
<td>dimensionless</td>
</tr>
<tr>
<td>Nucleon number</td>
<td>( A )</td>
<td>dimensionless</td>
</tr>
<tr>
<td>Planck constant</td>
<td>( h )</td>
<td>J·s</td>
</tr>
<tr>
<td>Planck constant/2(\pi)</td>
<td>( \hbar )</td>
<td>J·s</td>
</tr>
<tr>
<td>Proton number</td>
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<td>Proton rest mass</td>
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<td>Rotational constants</td>
<td>( A, B, C )</td>
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<td>Rotational term</td>
<td>( F )</td>
<td>m(^{-1})</td>
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<tr>
<td>Total angular momentum component</td>
<td>( m_j, m_f )</td>
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<tr>
<td>Total term</td>
<td>( T )</td>
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<td>Unified atomic mass unit</td>
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#### Chemical Kinetics

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<tr>
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<td>Energy of activation; Arrhenius or activation energy</td>
<td>( E, E_a, E_A )</td>
<td>J/mol, J·mol(^{-1})</td>
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<tr>
<td>Half-life</td>
<td>( t_{1/2} )</td>
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<tr>
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<td>( \text{s}^{-1} )</td>
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<tr>
<td>Rate constant, second order</td>
<td>( k )</td>
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<td>Rate of concentration change of substance B</td>
<td>( r_B )</td>
<td>( \text{mol}/(\text{m}^3 \cdot \text{s}) ), ( \text{mol} \cdot \text{m}^{-3} \cdot \text{s}^{-1} )</td>
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<tr>
<td>Rate of conversion</td>
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<tr>
<td>Rate of reaction</td>
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<tr>
<td>Relaxation time</td>
<td>( \tau )</td>
<td>( \text{s} )</td>
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<tr>
<td>Scattering angle</td>
<td>( \theta )</td>
<td>( \text{rad} )</td>
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<tr>
<td>Standard enthalpy of activation</td>
<td>( \Delta^\ddagger H^\circ, \Delta H^\ddagger )</td>
<td>( \text{J/mol}, \text{J} \cdot \text{mol}^{-1} )</td>
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<tr>
<td>Standard entropy of activation</td>
<td>( \Delta^\ddagger S^\circ, \Delta S^\ddagger )</td>
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<td>Standard Gibbs energy of activation</td>
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<tr>
<td>Standard internal energy of activation</td>
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<td>( \text{K} )</td>
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<td>( kT )</td>
<td>( \text{J} )</td>
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<tr>
<td>Volume of activation</td>
<td>( \Delta^\ddagger V, \Delta V^\ddagger )</td>
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## Electricity and Magnetism

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<td>( G )</td>
<td>( \text{S} )</td>
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<td>( \kappa )</td>
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<td>Electric charge</td>
<td>( Q )</td>
<td>( \text{C} )</td>
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<td>( I )</td>
<td>( \text{A} )</td>
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<td>( j )</td>
<td>( \text{A/m}^2, \text{A} \cdot \text{m}^{-2} )</td>
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<td>Electric dipole moment</td>
<td>( p, \mu )</td>
<td>( \text{C} \cdot \text{m} )</td>
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<td>( \text{C/m}^2, \text{C} \cdot \text{m}^{-2} )</td>
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<tr>
<td>Electric field strength</td>
<td>( E )</td>
<td>( \text{V/m, V} \cdot \text{m}^{-1} )</td>
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<tr>
<td>Electric potential</td>
<td>( V, \phi )</td>
<td>( \text{V, J}/\text{C, J} \cdot \text{C}^{-1} )</td>
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<tr>
<td>Electric potential difference</td>
<td>( U, \Delta V, \Delta \phi )</td>
<td>( \text{V} )</td>
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<tr>
<td>Electric resistance</td>
<td>( R )</td>
<td>( \Omega )</td>
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<td>( \text{A} \cdot \text{m}^2, \text{J}/\text{T, J} \cdot \text{T}^{-1} )</td>
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<td>( \Omega )</td>
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<td>( H )</td>
<td>( \text{A/m, A} \cdot \text{m}^{-1}, \text{H} )</td>
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<td>( \text{Wb} )</td>
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<td>( B )</td>
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<td>( B )</td>
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### Electricity and Magnetism—Continued

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<tr>
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<tr>
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<td>A/m, A·m(^{-1})</td>
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<td>Permeability</td>
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<td>H/m, H·m(^{-1})</td>
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<td>Permittivity</td>
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<td>F/m, F·m(^{-1})</td>
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<td>Polarization (of a particle)</td>
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<td>( \Omega·m )</td>
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<td>Self-inductance</td>
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<td>H</td>
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<tr>
<td>Voltage</td>
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### Electrochemistry

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<td>Diffusion rate constant</td>
<td>( k_d )</td>
<td>m/s, m·s(^{-1})</td>
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<td>Electric current</td>
<td>( I )</td>
<td>A</td>
</tr>
<tr>
<td>Electric current density</td>
<td>( j )</td>
<td>A/m(^2), A·m(^{-2})</td>
</tr>
<tr>
<td>Electric mobility</td>
<td>( u )</td>
<td>m(^2)/(V·s), m(^2)·V(^{-1})·s(^{-1})</td>
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<td>Electrode potential</td>
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<td>V</td>
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<td>Electrolytic conductivity</td>
<td>( \kappa )</td>
<td>S/m, S·m(^{-1})</td>
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<tr>
<td>Electromotive force (emf)</td>
<td>( E )</td>
<td>V</td>
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<tr>
<td>Elementary charge</td>
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<td>C</td>
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<tr>
<td>Faraday constant</td>
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<td>( E_{1/2} )</td>
<td>V</td>
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<td>Ionic strength</td>
<td>( I_c, I )</td>
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<td>molality basis</td>
<td>( I_m, I )</td>
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<td>Standard electromotive force (emf)</td>
<td>( E^\circ )</td>
<td>V</td>
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<tr>
<td>Surface charge density</td>
<td>( \sigma )</td>
<td>C/m(^2), C·m(^{-2})</td>
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### General Chemistry

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### Mechanics

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<td>J</td>
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<td>W</td>
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## NMR Spectroscopy

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<tr>
<td>direct (dipolar)</td>
<td>( D_{AB} )</td>
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<tr>
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</table>

## Polymer Chemistry

<table>
<thead>
<tr>
<th>NAME</th>
<th>SYMBOL</th>
<th>SI UNIT</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bulk modulus</td>
<td>( K )</td>
<td>Pa</td>
</tr>
<tr>
<td>Complex permittivity</td>
<td>( \varepsilon^* )</td>
<td>F/m, F·m(^{-1})</td>
</tr>
<tr>
<td>Crack-tip radius</td>
<td>( \rho_c )</td>
<td>m</td>
</tr>
<tr>
<td>Electrophoretic mobility</td>
<td>( \mu )</td>
<td>m(^2)·V(^{-1})·s(^{-1})</td>
</tr>
<tr>
<td>Flory–Huggins interaction parameter</td>
<td>( \chi )</td>
<td></td>
</tr>
<tr>
<td>Fracture strain</td>
<td>( \gamma_f, \varepsilon_f )</td>
<td>dimensionless</td>
</tr>
<tr>
<td>Fracture stress</td>
<td>( \sigma_f )</td>
<td>Pa</td>
</tr>
<tr>
<td>Glass-transition temperature</td>
<td>( T_g )</td>
<td>K</td>
</tr>
<tr>
<td>Modulus of elasticity</td>
<td>( E )</td>
<td>Pa</td>
</tr>
<tr>
<td>Tensile strength</td>
<td>( \sigma )</td>
<td>Pa</td>
</tr>
<tr>
<td>Viscosity</td>
<td>( \nu )</td>
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<tr>
<td>Volume fraction</td>
<td>( V_f )</td>
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<tr>
<td>Yield stress</td>
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</tr>
<tr>
<td>Young’s modulus</td>
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### Radiation

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</tr>
<tr>
<td>Absorption factor</td>
<td>$\alpha$</td>
<td>dimensionless, rad</td>
</tr>
<tr>
<td>Angle of optical rotation</td>
<td>$\alpha$</td>
<td>dimensionless</td>
</tr>
<tr>
<td>Angular frequency</td>
<td>$\omega$</td>
<td>s$^{-1}$, rad/s, rad·s$^{-1}$</td>
</tr>
<tr>
<td>Emissivity, emittance</td>
<td>$\varepsilon$</td>
<td>dimensionless</td>
</tr>
<tr>
<td>Frequency</td>
<td>$\nu$</td>
<td>Hz</td>
</tr>
<tr>
<td>Linear decadic absorption coefficient</td>
<td>$a$</td>
<td>m$^{-1}$</td>
</tr>
<tr>
<td>Molar decadic absorption coefficient</td>
<td>$\varepsilon_m$</td>
<td>m$^2$/mol, m$^2$·mol$^{-1}$</td>
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<td>Molar refraction</td>
<td>$R_m$</td>
<td>m$^3$/mol, m$^3$·mol$^{-1}$</td>
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<tr>
<td>Radiant energy</td>
<td>$Q, W$</td>
<td>J</td>
</tr>
<tr>
<td>Radiant intensity</td>
<td>$I$</td>
<td>W/sr, W·sr$^{-1}$</td>
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<tr>
<td>Radiant power</td>
<td>$P$</td>
<td>W</td>
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<tr>
<td>Refractive index</td>
<td>$n$</td>
<td>dimensionless</td>
</tr>
<tr>
<td>Speed of light</td>
<td>$c$</td>
<td>m/s, m·s$^{-1}$</td>
</tr>
<tr>
<td>Stefan–Boltzmann constant</td>
<td>$\sigma$</td>
<td>W/(m$^2$·K$^4$), W·m$^{-2}$·K$^{-4}$</td>
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<td>Transmittance</td>
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<tr>
<td>Wavelength</td>
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<tr>
<td>Wavenumber (in a vacuum)</td>
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### Space and Time

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<td>$A, S, A_S$</td>
<td>m$^2$</td>
</tr>
<tr>
<td>Cartesian space coordinates</td>
<td>$x, y, z$</td>
<td>m</td>
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<tr>
<td>Characteristic time interval</td>
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<td>s</td>
</tr>
<tr>
<td>Circular frequency</td>
<td>$\omega$</td>
<td>s$^{-1}$, rad/s, rad·s$^{-1}$</td>
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<tr>
<td>Diameter</td>
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<tr>
<td>Frequency</td>
<td>$\nu, f$</td>
<td>Hz</td>
</tr>
<tr>
<td>Height</td>
<td>$h$</td>
<td>m</td>
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<tr>
<td>Length</td>
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<td>m</td>
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<tr>
<td>Position vector</td>
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<td>m</td>
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<tr>
<td>Radius</td>
<td>$R$</td>
<td>m</td>
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<tr>
<td>Speed</td>
<td>$v, u, w, c$</td>
<td>m/s, m·s$^{-1}$</td>
</tr>
<tr>
<td>Thickness, distance</td>
<td>$d, \delta$</td>
<td>m</td>
</tr>
<tr>
<td>Time</td>
<td>$t$</td>
<td>s</td>
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<tr>
<td>Time constant</td>
<td>$\tau$</td>
<td>s</td>
</tr>
<tr>
<td>Velocity</td>
<td>$v, u, w, c$</td>
<td>m/s, m·s$^{-1}$</td>
</tr>
<tr>
<td>Volume</td>
<td>$V$</td>
<td>m$^3$</td>
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# Thermodynamics

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<tr>
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<td>$\lambda$</td>
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<tr>
<td>Affinity of a reaction</td>
<td>$A$</td>
<td>J/mol, J·mol$^{-1}$</td>
</tr>
<tr>
<td>Chemical potential</td>
<td>$\mu$</td>
<td>J/mol, J·mol$^{-1}$</td>
</tr>
<tr>
<td>Cubic expansion coefficient</td>
<td>$\alpha$</td>
<td>K$^{-1}$</td>
</tr>
<tr>
<td>Energy</td>
<td>$E$</td>
<td>J</td>
</tr>
<tr>
<td>Enthalpy</td>
<td>$H$</td>
<td>J</td>
</tr>
<tr>
<td>Entropy</td>
<td>$S$</td>
<td>J/K, J·K$^{-1}$</td>
</tr>
<tr>
<td>Fugacity</td>
<td>$f$</td>
<td>Pa</td>
</tr>
<tr>
<td>Gas constant</td>
<td>$R$</td>
<td>J/(K·mol), J·K$^{-1}$·mol$^{-1}$</td>
</tr>
<tr>
<td>Gibbs energy</td>
<td>$G$</td>
<td>J</td>
</tr>
<tr>
<td>Heat</td>
<td>$q, Q$</td>
<td>J</td>
</tr>
<tr>
<td>Heat capacity, molar</td>
<td>$C_m$</td>
<td>J/(K·mol), J·K$^{-1}$·mol$^{-1}$</td>
</tr>
<tr>
<td>Heat capacity at constant pressure</td>
<td>$C_p$</td>
<td>J/K, J·K$^{-1}$</td>
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<tr>
<td>Heat capacity at constant volume</td>
<td>$C_v$</td>
<td>J/K, J·K$^{-1}$</td>
</tr>
<tr>
<td>Helmholtz energy</td>
<td>$A$</td>
<td>J</td>
</tr>
<tr>
<td>Internal energy</td>
<td>$U$</td>
<td>J</td>
</tr>
<tr>
<td>Isothermal compressibility</td>
<td>$\kappa$</td>
<td>Pa$^{-1}$</td>
</tr>
<tr>
<td>Joule–Thomson coefficient</td>
<td>$\mu$</td>
<td>K/Pa, K·Pa$^{-1}$</td>
</tr>
<tr>
<td>Pressure, osmotic coefficient</td>
<td>$\Pi$</td>
<td>Pa</td>
</tr>
<tr>
<td>Pressure coefficient</td>
<td>$\beta$</td>
<td>Pa/K, Pa·K$^{-1}$</td>
</tr>
<tr>
<td>Specific heat capacity</td>
<td>$c$</td>
<td>J/(K·kg), J·K$^{-1}$·kg$^{-1}$</td>
</tr>
<tr>
<td>Surface tension</td>
<td>$\gamma$, $\sigma$</td>
<td>J/m$^2$, J·m$^{-2}$, N/m, N·m$^{-1}$</td>
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<tr>
<td>Temperature</td>
<td>$t, \theta$</td>
<td>°C</td>
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<td>thermodynamic</td>
<td>$T$</td>
<td>K</td>
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<tr>
<td>Viscosity</td>
<td>$\eta$</td>
<td>Pa·s</td>
</tr>
<tr>
<td>Work</td>
<td>$w, W$</td>
<td>J</td>
</tr>
</tbody>
</table>

## Transport Properties

<table>
<thead>
<tr>
<th>Name</th>
<th>Symbol</th>
<th>SI Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coefficient of heat transfer</td>
<td>$h$</td>
<td>W/(m$^2$·K), W·m$^{-2}$·K$^{-1}$</td>
</tr>
<tr>
<td>Diffusion coefficient</td>
<td>$D$</td>
<td>m$^2$/s, m$^2$·s$^{-1}$</td>
</tr>
<tr>
<td>Flux of a quantity $x$</td>
<td>$J_x$</td>
<td>$J$ varies</td>
</tr>
<tr>
<td>Heat flow rate</td>
<td>$\phi$</td>
<td>W</td>
</tr>
<tr>
<td>Kinematic viscosity</td>
<td>$\nu$</td>
<td>m$^2$/s, m$^2$·s$^{-1}$</td>
</tr>
<tr>
<td>Mass flow rate</td>
<td>$q_m$</td>
<td>kg/s, kg·s$^{-1}$</td>
</tr>
<tr>
<td>Mass-transfer coefficient</td>
<td>$k_d$</td>
<td>m/s, m·s$^{-1}$</td>
</tr>
<tr>
<td>Thermal conductivity</td>
<td>$\lambda$, $k$</td>
<td>W/(m·K), W·m$^{-1}$·K$^{-1}$</td>
</tr>
<tr>
<td>Thermal diffusion coefficient</td>
<td>$D_t$</td>
<td>m$^2$/s, m$^2$·s$^{-1}$</td>
</tr>
<tr>
<td>Thermal diffusivity</td>
<td>$a$</td>
<td>m$^2$/s, m$^2$·s$^{-1}$</td>
</tr>
<tr>
<td>Viscosity</td>
<td>$\eta$</td>
<td>Pa·s</td>
</tr>
<tr>
<td>Volume flow rate</td>
<td>$q_v$, $V$</td>
<td>m$^3$/s, m$^3$·s$^{-1}$</td>
</tr>
</tbody>
</table>
The Crystallographic Information File (CIF) is the internationally agreed on standard file format for the exchange of crystallographic information. Most major journals now require that crystal structure data for small molecules and inorganic compounds, obtained by single-crystal and powder diffraction analyses, be deposited as electronic CIFs as part of the manuscript submission process. A related format, the macromolecular CIF, or mmCIF, has been developed for data deposition with the Protein Data Bank. The CIF (and mmCIF) standard is maintained by the International Union of Crystallography (IUCr), and full information and leading references can be found at www.iucr.org/iucr-top/cif/.

Important sources of three-dimensional crystal structure data, including data in CIF or mmCIF format, are the following:

- The Cambridge Crystallographic Data Centre produces the Cambridge Structural Database (http://www.ccdc.cam.ac.uk/products/csd/), which covers organic and metal-organic small-molecule crystal structures.
- CRYSTMET (http://www.tothcanada.com/) contains data for metals, intermetallics, and alloys.
- FIZ Karlsruhe produces the ICSD (http://www.fiz-informationsdienste.de/en/FG/Kristall/index.html), which contains information on inorganic crystal structures.
- The Nucleic Acid Database (http://ndbserver.rutgers.edu/) contains data on oligonucleotides.
- The Protein Data Bank (http://www.rcsb.org/pdb/) contains biological macromolecular structure data.

CIF principles are simple. Every data item is represented by a unique data name followed by its associated data value. Data items are described in an electronic dictionary that defines meaning, usage, and (where appropriate) permitted values or ranges of values. Data names start with an underscore (underline) character, and data values can be any type of string (text, numeric, or mixed), ranging from a single character to many lines of text. Data values are delimited by spaces, double or single quotes, or pairs of lines beginning with a semicolon (to delimit
Chapter 13: Conventions in Chemistry

➤ 285

multiline data items). Related data items, such as those that relate to an individual crystal structure, are grouped together in a data block. The start of a block is designated by the string data_ prefixing the name of the block, and the end of a block is recognized by another data_record introducing a new block, or by the end of the file. A complete CIF may contain any number of data blocks, each reporting an individual crystal structure, and these may be preceded by a data block containing items (such as author names and contact details) that are common for all structures in the complete CIF.

These basic principles, together with the data names in the CIF standard, make the CIF human readable, as illustrated below:

```cif
data_structure_1
_cell_length_a   5.959(1)
_chemical_formula_moiety 'C23 H36 O7'
_publ_contact_author
;
Dr J. Smith
Department of Chemistry
University of Nowhere
Nowhere
Anystate 20761
USA
;

If a data name is preceded by loop_, then a series of values can be associated with that name, e.g., _symmetry_equiv_pos_as_xyz. A series of data values can also be grouped together under different data names using the loop_construct, as in the example below, which shows a loop containing the atom labels and x,y,z-coordinates for four atoms. Here, the data names can be regarded as the column headings in a conventional printed table.

```cif
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
I1 0.26639(7) 0.61557(3) 0.94292(3)
I2 0.64548(7) 0.36489(3) 0.56299(3)
P3 0.0438(2) 0.27607(11) 0.74432(13)
O1 -0.0989(7) 0.2488(3) 0.6619(4)
```

The crystallographic part of a CIF is generated automatically by the software package used for structure refinement. However, the software can only output data items that it knows about, i.e., those items that are input to or are generated by the refinement process, or which can be generated reliably from these data.

This is seldom sufficient for journal submission, where additional data, such as author names and contact details, and other chemical or crystal property
information are almost always required. Because these additional requirements
will vary from journal to journal, authors should consult the author guidelines
for the journal of their choice to ensure that they submit files that conform to
the publisher’s requirements.

Although the CIF can be edited using standard text editors, this is not rec-
ommended because the strict syntax, if broken in any small way, renders the
file unreadable by application software. To solve the editing issue, a number of
stand-alone CIF editors have been written. For example, the enCIFer program is
available for free download from the Cambridge Crystallographic Data Centre
Web site (http://www.ccdc.cam.ac.uk). The program will handle single-block or
multiblock CIFs and has a graphical interface that permits the following:

- location, display, and correction of syntax or format violations using the
current CIF dictionary;
- spreadsheet representation of looped data items;
- editing and/or addition of individual or looped data items;
- addition of certain standard information (basic bibliographic and/or
  property information) via two data entry wizards; and
- three-dimensional visualization of the structure(s) contained in the CIF.

The IUCr Web site (http://www.iucr.org/iucr-top/cif/) lists other software
that can be used to manipulate or visualize CIF content. Most importantly, they
maintain a Web-based service that provides a classified validation report on any
format-compliant CIF. This service can be accessed at http://checkcif.iucr.org./
CheckCIF reports can be lengthy, but it is wise to scan them carefully, particu-
larly the most serious Class A alerts. Journal editors and their referees will often
indicate the types of alerts that they would normally expect to be fixed by the
authors before publication.
This chapter presents style conventions for citing references within a manuscript and for listing complete reference citations. Many of the references in the examples were created to illustrate a style point under discussion; they may not be real references.

Citing References in Text

In ACS publications, you may cite references in text in three ways:

1. By superscript numbers, which appear outside the punctuation if the citation applies to a whole sentence or clause.

   Oscillation in the reaction of benzaldehyde with oxygen was reported previously.\(^3\)

2. By italic numbers in parentheses on the line of text and inside the punctuation.

   The mineralization of TCE by a pure culture of a methane-oxidizing organism has been reported (6).

3. By author name and year of publication in parentheses inside the punctuation (known as author–date).

   The primary structure of this enzyme has also been determined (Finnegan et al., 2004).

In ACS books, all three of these systems are used, depending on the subject matter and series. Table 14-1 lists the referencing systems used by the ACS journals currently in print.
<table>
<thead>
<tr>
<th>Name as Registered in the U.S. Patent and Trademark Office</th>
<th>Referencing Style&lt;sup&gt;a&lt;/sup&gt;</th>
<th>CASSI Abbreviation</th>
<th>2006 Vol.</th>
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<tr>
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<td>ACS Chem. Biol.</td>
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<td>review issues</td>
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<td>2</td>
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<tr>
<td>Chemical &amp; Engineering News</td>
<td></td>
<td>Chem. Eng. News</td>
<td>84</td>
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<td>Chemical Research in Toxicology</td>
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<td>Chem. Res. Toxicol.</td>
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<td>Industrial &amp; Engineering Chemistry Research</td>
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<td>Ind. Eng. Chem. Res.</td>
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</tr>
<tr>
<td>Inorganic Chemistry</td>
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<td>Inorg. Chem.</td>
<td>45</td>
</tr>
<tr>
<td>Journal of Agricultural and Food Chemistry</td>
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<td>J. Agric. Food Chem.</td>
<td>54</td>
</tr>
<tr>
<td>Journal of the American Chemical Society</td>
<td>1</td>
<td>J. Am. Chem. Soc.</td>
<td>128</td>
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<tr>
<td>Journal of Chemical and Engineering Data</td>
<td>1</td>
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<tr>
<td>Journal of Chemical Information and Modeling</td>
<td>1</td>
<td>J. Chem. Inf. Model.</td>
<td>46</td>
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<td>Journal of Combinatorial Chemistry</td>
<td>1</td>
<td>J. Comb. Chem.</td>
<td>8</td>
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<td>Journal of Medicinal Chemistry</td>
<td>1</td>
<td>J. Med. Chem.</td>
<td>49</td>
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<td>Journal of Natural Products</td>
<td>1</td>
<td>J. Nat. Prod.</td>
<td>69</td>
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<td>Journal of Proteome Research</td>
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<td>J. Proteome Res.</td>
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</tbody>
</table>

<sup>a</sup>Reference style 1 uses superscript numbers, and 2 uses italic numbers in parentheses on the line of the text.
In all three systems, the author’s name may be made part of the sentence. In such cases, in the author–date system, place only the year in parentheses.

The syntheses described by Fraser\(^8\) take advantage of carbohydrate topology.

Jensen\((3)\) reported oscillation in the reaction of benzaldehyde with oxygen.

According to Harris (2003), drug release is controlled by varying the hydrolytic stability of the ester bond.

With numerical reference citations, start with 1 and number consecutively throughout the paper, including references in text and those in tables, figures, and other nontext components. If a reference is repeated, do not give it a new number; use the original reference number.

Whenever authors are named, if a reference has two authors, give both names joined by the word “and”. If a reference has more than two authors, give only the first name listed, followed by “et al.” Do not use a comma before et al.; always use a period after al.

Allison and Perez\(^{12}\)
Johnson et al.\((12)\)
(O’Brien and Alenno, 2005)
(Bachrach et al., 2004)

To cite more than one reference by the same principal author and various coauthors in one of the numerical citation systems, use the principal author’s name followed by “and co-workers” or “and colleagues”.

Pauling and co-workers\(^{10,11}\)
Cram and colleagues\((27–29)\)

When citing more than one reference at one place by number in one of the numerical systems, list the numbers in ascending order and separate them by commas (\textit{without} spaces as superscripts, \textit{with} spaces on line), or if they are part of a consecutive series, use an en dash to indicate a range of three or more.

in the literature\(^2,5,8\)
were reported\(^3–5,10\)

in the literature \((2, 5, 8)\)
were reported \((3–5, 10)\)

When citing more than one reference at one place by the author–date system, list them alphabetically according to the first author’s name, followed by a comma and the year. Use a semicolon to separate individual references.

(Axelrod, 2003; Cobbs and Stolman, 2005; Gerson et al., 2001)
When citing more than one reference by the same author at one place by the author–date system, do not repeat the name. List the name followed by the year of each of the references in ascending order; separate the years by commas. If an author has more than one reference in the same year, add lowercase letters to the years to differentiate them. Add letters to all of the years, for example, 2005a, 2005b, etc., not 2005, 2005a, etc. (The references in the list will need to be listed the same way, for example, 2005a, 2005b.

(Knauth, 2005a, 2005b)
(Fordham, 2004; Fordham and Rizzo, 2004)

Cite the reference in a logical place in the sentence.

recent investigations (cite)
other developments (cite)
was reported (cite)
as described previously (cite)
previous results (cite)
were demonstrated (cite)
a molecular mechanics study (cite)
Marshall and Levitt’s approach (cite)
the procedure of Lucas et al. (cite)

Style for Reference Lists

Authors are responsible for the accuracy and completeness of all references. Authors should check all parts of each reference listing against the original document.

A reference must include certain minimum data:

- Periodical references must include the author names, abbreviated journal title, year of publication, volume number (if any), and initial page of cited article (the complete span is better).
- Book references must include the author or editor names, book title, publisher, city of publication, and year of publication.
- For material other than books and journals, sufficient information must be provided so that the source can be identified and located.

In lists, references always end with a period.

Table 14-2 provides sample references for common reference types.
Periodicals

RECOMMENDED FORMATS

Author 1; Author 2; Author 3; etc. Title of Article. Journal Abbreviation Year, Volume, Inclusive Pagination.
Author 1; Author 2; Author 3; etc. Journal Abbreviation Year, Volume, Inclusive Pagination.

The journal Biochemistry is an exception. Consult this journal’s instructions to authors for the correct format.

Author Name Field

Include all author names in a reference citation. With multiple authors, separate the names from one another by semicolons. Always end the author field with a period (exception: Biochemistry). List the names in inverted form: surname first, then first initial, middle initial, and qualifiers (Jr., II). Some publications list the first 10 authors followed by a semicolon and et al.; check the guidelines.

Cotton, F. A.
Basconi, J.; Lin, P. B.
Chandler, J. P., III; Levine, S. M.
Schafer, F. W., Jr.
Fishman, W., II.

Farhataziz. (a single name is uncommon, but does occur; no period in Biochemistry)

Inderjit; Fontana, M. J. (the first author has a single name)

Article Title Field

Article titles are not essential in reference citations, but they are considered desirable to highlight the contents of a paper and facilitate location in reference libraries. Some ACS publications include the article title in journal references, and some do not; check the publication itself. Article titles are set in roman type without quotation marks and end with a period (or a question mark if that is part of the title). In ACS journals, capitalization follows that of the original publication; in other publications, the main words are capitalized.


Journal Abbreviation Field

The journal name is an essential component of a periodical reference citation.Abbreviate the name according to the Chemical Abstracts Service Source Index
## Table 14-2. Common Types of References with Examples

<table>
<thead>
<tr>
<th>Reference Type</th>
<th>See Pages</th>
<th>Example</th>
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<tr>
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</tr>
<tr>
<td><strong>Personal communications</strong></td>
<td>315–316</td>
<td>Henschler, L. X. University of Minnesota, Minneapolis, MN. Personal communication, 2001.</td>
</tr>
<tr>
<td><strong>Online Periodicals</strong></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table 14-2. Common Types of References with Examples—Continued

<table>
<thead>
<tr>
<th>Reference Type</th>
<th>See Pages</th>
<th>Example</th>
</tr>
</thead>
</table>

Other Online Sources

| Electronic mail messages                   | 322       | Solla, L. R. Cornell University, Ithaca, NY. Personal communication, 2005. |
The ACS Style Guide

(CASSI), and italicize it. One-word journal names are not abbreviated (e.g., *Biochemistry*, *Macromolecules*, *Nature*, *Science*). No punctuation is added to end this field; thus, a period will be there with an abbreviation but not with a spelled-out word.

*CASSI* and its quarterly supplements provide an extensive list of recommended journal abbreviations. Appendix 14-1 lists *CASSI* abbreviations for more than 1000 of the most commonly cited journals. ACS publication names, their abbreviations, and their volume numbers for 2006 are given in Table 14-1. Note that, in some cases, the word “the” is part of the title.

Sometimes journal names change. Authors should use the abbreviation of the journal title that was in use at the time the article was published. *CASSI* lists the journal titles and the range of years during which the title was being used.

**Information Found in CASSI**

Entries are arranged in *CASSI* alphabetically according to the abbreviated form of the title. Abbreviations are based on the standards of the International Organization for Standardization (ISO). Recommended abbreviations are indicated in boldface type. See Appendix 14-2 for a sample *CASSI* entry with a description of each element in an entry.

**Using CASSI Abbreviations**

➤ The boldface components of the publication title form the abbreviated title. Use a period after each abbreviation, and maintain the punctuation shown in *CASSI*.

*Journal of Polymer Science, Part A: Polymer Science*


➤ Maintain the word spacing shown in *CASSI*, except for D.C., N.Y., U.K., U.S., and U.S.A.

*Analyst (Cambridge, U.K.)*

*Anesth. Analg. (Hagerstown, MD, U.S.)*

*Ann. N.Y. Acad. Sci.*


*Science (Washington, DC, U.S.)*

➤ Use a terminal period only if the last word of the periodical title is abbreviated.

*International Journal of Nanoscience*

*Int. J. Nanosci.* (last word is abbreviated; period is used)

*Journal of Controlled Release*

*J. Controlled Release* (last word is not abbreviated; no period is used)
If the periodical abbreviation in CASSI shows a hyphen with spaces on both sides, change the hyphen to an em dash closed up on each side.

Annual Technical Conference - Society of Plastics Engineers

If a boldface n precedes the volume number in CASSI, use the abbreviation “No.” before the volume number in italics in the entry.

British Medical Journal ... n6372 1983

Include all the information shown for volume in italics, especially for references to government publications and reports.

Los Alamos National Laboratory, [Report] LA (United States) ... LA-14240-SR 2005

Exceptions to the Rules of CASSI Abbreviations

Strict rules for CASSI abbreviations can be modified for periodicals whose titles include multiple parts, sections, and series.

ABBREVIATION


ACCEPTABLE VARIATION The section title need not be named:


ACCEPTABLE VARIATION The section can be indicated by the volume number:


For some periodicals whose CASSI abbreviation includes a place of publication, you need not add the place of publication unless its omission would create ambiguity. If CASSI lists only one journal with a given main title, there is no ambiguity in omitting the place of publication.

USE NOT NECESSARILY

Clin. Chem.  
Nature  
Science  
Science (Washington, DC, U.S.)

In contrast, omission of the place of publication would create ambiguity for different journals having the same main title.

Transition Met. Chem. (Dordrecht, Neth.)  
Transition Met. Chem. (N.Y.)
Year of Publication Field

The year of publication is essential information in a periodical citation. The year is set in boldface type, followed by a comma in boldface type.

Publication Volume Field

The volume number is important information and is recommended for all periodical citations; it is essential for publications having more than one volume per year (such as the *Journal of Chemical Physics*). The volume number is set in italic type and is separated from the pagination information by a comma, which is set in italic type.

➤ For periodicals in which each issue begins with page 1, include issue information (either the number or the date) in the publication volume field. Issue information is set in roman type, enclosed in parentheses, and spaced from the volume number, which it directly follows.

**ISSUE NUMBER**


**DATE OF ISSUE**


➤ For publications that have supplements, the following form is recommended.


➤ For journals that have no volume numbers, include issue numbers, especially when the pagination of each issue begins with page 1. Use the following form. Note that the issue number is not italicized.


Pagination Field

Pagination is an essential element of a reference citation. The complete page range is preferable, but initial page numbers are acceptable.

➤ In page spans, use all digits, closed up, with no commas or spaces.

2–15
44–49
103–107

1376–1382
2022–2134
11771–11779
You may also indicate pagination in reference citations by “f” or “ff”, which mean “and following” page or pages, respectively. The f or ff is set in roman type and is spaced from the preceding number:

- 60 f (indicates page 60 and the page following—pages 60 and 61)
- 60 ff (indicates page 60 and pages following)
- 58–60 ff (indicates pages 58 through 60 and pages following—essentially the same as 58 ff except that the three pages enumerated contain the most pertinent information and other relevant information is scattered on the rest of the pages)

The pagination field may also include terms such as “and references therein” and similar expressions (especially in references to review articles). This phrase follows the page numbers and is not separated by a comma.


Some publications use article numbering, rather than page numbering, where each article starts on page 1. Use the article number in the pagination field.


Use of Punctuation To Indicate Repeating Fields of Information

The choice of what punctuation to use to indicate repeating fields of information depends on whether the publication will appear strictly in print or on the Web. For publications that will appear in both print and on the Web, use the rules for Web publications.

In references that will appear only in print publications, use a semicolon, a comma, or a period to indicate repeating information.

1. Same authors in multiple publications:


2. Same authors in multiple publications, but with letters to separate the references (the semicolon from the previous example is changed to a period):


3. Same authors of multiple articles in the same journal:


When the year and volume are the same:

When the year is the same but the volumes are different:


In references that will appear only in Web publications, provide complete references so that the references can be properly linked. If two or more references with the same authors are cited, it is not acceptable to combine them into a single reference.

1. Same authors in multiple publications:


2. Same authors in multiple publications, but with letters to separate the references:


3. Same authors of multiple articles in the same journal:


The same principle holds no matter what information is being repeated: provide each reference in its entirety. Do not use the Latin terms ibid. (in the same place) or idem (the same).

**References to Chemical Abstracts**

Use a semicolon to separate the periodical citation from a reference to its abstract (*Chemical Abstracts*).


*Chemical Abstracts* routinely contains more than one abstract per page. The method of distinguishing which abstract was being cited has changed over the years. Three variations are worth noting.

1. The column (two columns per page) in which the abstract occurs followed by a superscript number:

   *Chem. Abstr.* 1946, 40, 4463⁸. (This is the eighth abstract in column 4463.)

2. The column (two columns per page) in which the abstract occurs followed by a letter, either on the line or superscript (generally italic):
3. The abstract number itself followed by an online letter (roman), often a computer check character:

Chem. Abstr. 1989, 110, 8215j. (This is abstract number 8215.)

**Special Situations**

➤ You may treat Beilstein references as periodical references.

Beilstein, 4th ed. 1950, 12, 237.

➤ Cite journals published in a foreign language either by the actual non-English title or by a translated form.

*Nippon Ishikai Zasshi* or *J. Jpn. Med. Assoc.*


➤ When citing an article printed in the English translation of a foreign-language journal, include reference to the original article, if possible, and use a semicolon to separate the two citations.


➤ Separate two or more companion publications with a semicolon.


**NonScientific Magazines and Newspapers**

**Recommended Format**

Author 1; Author 2; Author 3; etc. Title of Article. *Title of Periodical*, Complete Date, Pagination.

For nonscientific magazines and other periodicals that are not abstracted by Chemical Abstracts Service, give the authors’ names in inverted form ending with a period, the article title in roman type with main words capitalized and ending with a period, the full magazine title in italic type followed by a comma in italic type, the complete date of the issue (see pp 160–161 about dates) ending with a comma, and the pagination.

Books

Some ACS publications include the chapter title in book references, and some do not; check the publication itself. Also, consult the instructions to authors in *Biochemistry* for exceptions to the format presented here and elsewhere in this chapter.

**RECOMMENDED FORMATS FOR BOOKS WITHOUT EDITORS**

Author 1; Author 2; Author 3; etc. Chapter Title. *Book Title*, Edition Number; Series Information (if any); Publisher: Place of Publication, Year; Volume Number, Pagination.

Author 1; Author 2; Author 3; etc. *Book Title*; Series Information (if any); Publisher: Place of Publication, Year; Volume Number, Pagination.

When a book has authors and no editors, it means either that the entire book was written by one author or that two or more authors collaborated on the entire book.


**RECOMMENDED FORMATS FOR BOOKS WITH EDITORS**

Author 1; Author 2; Author 3; etc. Chapter Title. In *Book Title*, Edition Number; Editor 1, Editor 2, etc., Eds.; Series Information (if any); Publisher: Place of Publication, Year; Volume Number, Pagination.

Author 1; Author 2; Author 3; etc. In *Book Title*, Edition Number; Editor 1, Editor 2, etc., Eds.; Series Information (if any); Publisher: Place of Publication, Year; Volume Number, Pagination.

When a book has editors, it means that different authors wrote various parts of the book independently of each other. The word “In” before the book title indicates that the authors mentioned wrote only a part of the book, not the entire book.


If the book as a whole is being referenced, the author names might not appear.

Author Name Field

➤ Separate the names of multiple authors by semicolons, and always end the author field with a period (except in Biochemistry). List names in inverted form: surname first, then first initial, middle initial, and qualifiers (Jr., II).

➤ If a book has no primary authors because each chapter was written by a different author, you may place the editor names in the author name field (especially for lists in alphabetical order). Separate editor names by commas, and in this case, the period after the abbreviation Ed. or Eds. terminates the field.


➤ A book might have no named authors because it was compiled by a committee or organization. These books are discussed under the section “Works Written by an Organization or a Committee”, p 307.

Chapter Title Field

Chapter titles are not essential, but they are considered desirable components in reference citations because they highlight the contents of a paper and facilitate its location in reference libraries. Chapter titles are set in roman type and end with a period.


Book Title Field

Book titles are essential elements in book reference citations. In general, book titles should not be abbreviated. They are set in italic type and are separated from the next field of the reference by a semicolon, which is set in italic type.

➤ The edition number (in ordinal form) and the abbreviation “ed.” follow the book title, set off by an italic comma; they are set in roman type. The edition information is separated from the next field of the reference by a semicolon.

Reagent Chemicals, 10th ed.;

➤ When both authors and editors are given, use the word “In” (set in roman type) immediately before the title of the book to indicate that the cited authors wrote only part of the book.
Editor Name Field

For books with editors, list the names of the editors, after title and edition information, in inverted form as described in the section “Author Name Field”, separated from one another by commas. The names are denoted as editors by including the abbreviation “Eds.” or “Ed.” after the final name. The editor field is set in roman type and ends with a semicolon (unless it is used in the author field location).


In books that have no primary authors, the names of the editors may appear in either the author name field (especially for lists in alphabetical order) or the editor name field. When the editor names appear in the author name field, they are separated by commas and the field ends with a period.


Publication Information Field

The name of the publisher, place of publication, and year of publication are essential elements in a book reference.

Name of Publisher

Check the title page, front and back, for the publisher’s name and location. Names and addresses of publishers are also listed in Chemical Abstracts Service Source Index, 1907–2004 Cumulative, pp 211–391.

➤ Generally, do not abbreviate publishers’ names.

American Chemical Society, not Am. Chem. Soc. or ACS
American Ceramic Society, not Am. Ceram. Soc.

EXCEPTION You may use well-known acronyms or abbreviations created by the publishers themselves.

AIChE or American Institute of Chemical Engineers
ASTM or American Society for Testing and Materials
IUPAC or International Union of Pure and Applied Chemistry
In some publisher’s names, words such as Co., Inc., Publisher, and Press are not essential.


Expanded names are also not essential.

John Wiley & Sons or John Wiley or Wiley

It is not necessary to repeat the publisher’s name for a book compiled by the organization that published it.


Place of Publication
For the place of publication, give the city and state for U.S. cities or the city and country for all others. The country or state is not needed if the city is considered a major city in the world and could not be confused easily with other cities of the same name (e.g., London, Paris, New York, and Rome). Use the two-letter postal abbreviations (listed in Chapter 10) for states. Spell out names of countries unless they have standard abbreviations, such as U.K. for United Kingdom.

Boca Raton, FL Elmsford, NY Springfield, IL
Cambridge, MA Englewood Cliffs, NJ Springfield, MA
Cambridge, U.K. London Washington, DC
Chichester, U.K. New York

Year of Publication
In book references, the year is set in lightface (not bold) roman type, following the place of publication. Terminate the field with a period or with a semicolon if further information is given.


Volume and Pagination Field

Volume Information

The volume field contains specific information, such as volume number and chapter number. Use the following abbreviations and spelled-out forms with the capitalization, spelling, and punctuation shown:

Abstract
Chapter
If a volume or part number refers to the volume or part of an entire series of books, this information is placed where a series number would normally appear and not in the volume field for the specific book being cited.


If the book or set of books as a whole is the reference, do not include individual volume information.


**Pagination Information**

If you are citing a chapter, the complete page range is best, but initial page numbers are acceptable. Pagination may also be indicated by “f” or “ff” notation (meaning “and following” page or pages, respectively). The f or ff is set in roman type and is spaced from the preceding number. These points are illustrated under the “Pagination Field” heading for periodicals.

Pagination information is set in roman type and ends with a period, except when miscellaneous information follows it, in which case it should end with a semicolon (see the next section). Use the abbreviations “p” and “pp” to indicate single and multiple pages, respectively.

- p 57
- p 93 f
- pp 48–51
- pp 30, 52, 76
- pp 30, 52, 76 ff

If the book as a whole is the reference, page numbers need not be given.
**Miscellaneous Information**

If you wish to include additional information about a book that is important for the reader to know, you may add it at the end of the reference with or without parentheses, append it to the title in parentheses before the semicolon, or place it between the title and the publisher.


**Special Situations**

- *Organic Syntheses* collective volumes should be treated as books.


<table>
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<th>COLLECTIVE VOLUME NO.</th>
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<tr>
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</tr>
<tr>
<td>1943</td>
<td>II</td>
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<td>VI</td>
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<td>1990</td>
<td>VII</td>
</tr>
<tr>
<td>1993</td>
<td>VIII</td>
</tr>
<tr>
<td>1998</td>
<td>IX</td>
</tr>
<tr>
<td>2004</td>
<td>X</td>
</tr>
</tbody>
</table>

*Organic Syntheses, Cumulative Indices for Collective Volumes I–VIII* was published in 1995. Beginning with Volume 82, each volume of *Organic Syntheses* is planned to be published online on orgsyn.org in installments about every three months, with printed volumes appearing annually.

- For references to the *Kirk-Othmer Encyclopedia*, include the article title followed by a period, similar to the citation of a chapter title.

**Series Publications**

Publications such as book series that are periodical in nature but are not journals may be styled as either books or journals. CASSI lists every document abstracted and indexed by the Chemical Abstracts Service; hence, book titles are included and abbreviated. Key words to look for with these types of publications include “Advances”, “Methods”, “Progress”, and “Series”.

**RECOMMENDED FORMAT FOR CITATION AS A BOOK**

Author 1; Author 2; Author 3; etc. In Title; Editor 1, Editor 2, Eds.; Series Title and Number; Publisher: Place of Publication, Year; Pagination.

➤ In book format, use the regular citation format for a book reference, but include information pertaining to the series. The series title is spelled out and set in roman type.


➤ If a volume or part number is given for a series of books instead of a series number, cite this information where a series number would normally appear.


➤ As for any book, you may cite specific chapters.


➤ In journal format, the series title is used as a journal title, abbreviated according to CASSI and italicized, and the series number is used as a journal volume number.

**RECOMMENDED FORMAT FOR CITATION AS A JOURNAL**

Author 1; Author 2; Author 3; etc. Abbreviation Year, Volume, Pagination.


Works Written by an Organization or a Committee

An organization or a committee may be the author of a book or periodical article. Acronyms for very well known organizations may be used. It is not necessary to repeat the publisher’s name for a work compiled by the organization that published it.

BOOK FORMAT


PERIODICAL FORMAT


Meetings and Conferences

References to work presented at conferences and meetings must be treated on a case-by-case basis. At least three types of citations are possible:

1. Full citations of published abstracts and proceedings. The format resembles that of a book citation.
2. CASSI citations of published abstracts and proceedings. The format is that of a periodical citation.
3. References to oral presentations, posters, or demonstrations at technical meetings, possibly accompanied by handouts or brochures. These references contain no publication information.

Full Citations

RECOMMENDED FORMAT

Author 1; Author 2; Author 3; etc. Title of Presentation. In *Title of the Collected Work*, Proceedings of the Name of the Meeting, Location of Meeting, Date of Meeting; Editor 1, Editor 2, etc., Eds.; Publisher: Place of Publication, Year; Abstract Number, Pagination.

The format resembles that of a book citation. The title field, however, includes additional information on the meeting title, location, and dates. The actual title
of the book (collected work) is set in italic type and is separated from the meeting information by a comma. The information on meeting location is set in roman type, but it is not repeated if it is included in the book title. The entire field ends with a semicolon.


Abstracts are slightly different in that they usually do not have editors. The word “in” is not used before the book title.


When the phrase “Proceedings of” is part of the reference, include the publisher and place of publication. When a society sponsors a meeting, the society is assumed to be the publisher. If the place of the meeting and the place of publication are the same, additional publisher and place information is not required. However, many organizations such as the ACS sponsor meetings in various cities.


**CASSI Citations**

Proceedings and abstracts of meetings and conferences are indexed in CASSI. The reference format follows that for periodicals.


CASSI gives the number of a meeting in ordinal form. Convert this number to an italic cardinal number, and use it as the volume number in the citation, unless CASSI has already indicated another volume number.

Journal format can be used for references to preprint papers.


**Material That Has No Publication Information**

**RECOMMENDED FORMATS**

Author 1; Author 2; Author 3; etc. Title of Presentation (if any). Presented at Conference Title, Place, Date; Paper Number.

List the data concerning the conference (name, place, and date) separated by commas and followed by a semicolon and the paper number (if any). The entire citation is set in roman type.
Dizman, B.; Elasri, M. O.; Mathias, L. J. Presented at the 227th National Meeting of the American Chemical Society, Anaheim, CA, March 28–April 1, 2004; Paper POLY 229.

**Theses**

**RECOMMENDED FORMATS**

Author. Title of Thesis. Level of Thesis, Degree-Granting University, Location of University, Date of Completion.

References to theses should be as specific as practical, including, at a minimum, the degree-granting institution and date.


**Author Name Field**

Cite the name in inverted form: surname first, then first initial, middle initial, and qualifiers (Jr., II). End the field with a period.

**Title Field**

Thesis titles are not essential, but they are informative. They are set in roman type and end with a period.


**Thesis Level Field**

Work done at a master’s level is often called a thesis. Work toward the Ph.D. (doctor of philosophy) may be called a thesis or a dissertation, depending on the policy of the degree-granting institution. The following abbreviations are standard for U.S. degrees. Many variations exist for degrees from institutions of other countries.
The name of the degree-granting university is the minimum requirement for an acceptable citation. You should also include the city and state or city and country. Use the two-letter postal abbreviations for states. Spell out names of countries unless they have standard abbreviations, such as U.K. for United Kingdom.


Indicate the date the thesis was completed by year only; month and year; or month, day, and year.


The minimum data required for an acceptable citation are the name(s) of the patent owner(s), the patent number, and the date. Ensure that the patent stage (Patent, Patent Application, etc.) is indicated and that the pattern of the number (e.g., spaces, commas, dashes) follows that of the original patent document. If possible, include the title and the Chemical Abstracts reference (preceded by a semicolon) as well.

Chapter 14: References


**Government Publications**

Publications of the U.S. government and those of state and local governments can be pamphlets, brochures, books, maps, journals, or almost anything else that can be printed. They may have authors or editors, who may be individuals, offices, or committees, or the author may not be identified. They are published by specific agencies, but they are usually (though not always) available through the Government Printing Office rather than the issuing agency. To enable others to find the publication, the American Library Association suggests that you include as much information as possible in the citation. The following are examples of the most commonly cited types of references.

**Publications of Federal Government Agencies**

**Recommended Format**

Author 1; Author 2; etc. Chapter Title. *Document Title; Government Publication Number; Publishing Agency: Place of Publication, Year; Pagination.*

The format resembles that of a serial publication in book format. Include as much information as possible.


Author Name Field
Include all author names. With multiple authors, separate the names from one another by semicolons. Always end the author field with a period. List the names in inverted form: surname first, then first initial, middle initial, and qualifiers (Jr., II). Some publications list the first 10 authors followed by a semicolon and “et al.”

Chapter Title Field
Chapter titles are set in roman type and end with a period.

Document Title Field
Treat the formal title of the document as the title of a book. These titles are set in italic type and are separated from the next component of the reference by a semicolon, which is set in italic type.

Government Publication Number Field
The government publication number, also called an agency report number, is important because it is unique to the publication and because some indexing services provide access by these numbers. These numbers (or number–letter combinations) are usually printed somewhere on the cover or title page of the document and are sometimes identified as a “report/accession number”. Treat a report number the same as a series number; that is, it follows the book title, ends with a semicolon, and is set in roman type.

Publishing Agency Field
The publishing agency field may take on added complexity in government publications. Often, the office or agency issuing the report as well as the Government Printing Office must be cited. The order is department or agency, administration or office, and finally U.S. Government Printing Office, all separated by commas and set in roman type. The field ends with a colon.

Place of Publication Field
For the U.S. Government Printing Office, it is always Washington, DC. The field ends with a comma preceding the date of publication.

Year of Publication Field
The year of publication is set in roman type and ends with a semicolon if it is followed by pagination information. It ends with a period if it is the last field.

Pagination Field
The page numbers are set in roman type and end with a period, unless miscellaneous material is appended to the reference.
Alternative Format

Government agency references can also be given with CASSI abbreviations. In that case, the format is the same as for periodicals.


Other Federal Publications

Federal Register

The Federal Register is a periodical and is treated as such in citations.


Code of Federal Regulations


U.S. Code


U.S. Laws

Treat the name of the law as a chapter title (roman, terminated with a period). No publisher name is needed. The number and date of the law are separated by a comma. If additional publication information is given, it is preceded by a semicolon.


State and Local Government Publications

RECOMMENDED FORMAT

Author 1; Author 2; etc. Chapter Title. Document Title; Publication Number or Type; Publishing Agency: Place of Publication, Date; Pagination.

Annual Report 2004: Moving Forward; Santa Barbara County Air Pollution Control District: Santa Barbara, CA, 2005.
Technical Reports and Bulletins

Technical reports and bulletins come in many forms. Examples of some of these have already been presented. Many are in-house publications, and some are government publications. Others are reports of work in progress. The publication itself may include a phrase alluding to its status as a technical report or technical bulletin, but it may also simply be called a report or bulletin. Include whatever information is available, following the format shown for the word “Report”, “Report No.”, etc. Document titles are set in italic type.

RECOMMENDED FORMAT

Author 1; Author 2; etc. Title of Report or Bulletin; Technical Report or Bulletin Number; Publisher: Place of Publication, Date; Pagination.


Data Sets

Data sets are compilations of data, such as spectra or property tables. These data sets are often published serially as loose-leaf services, but the content is not always organized in chapters as in other serial publications. The citation of a serial data set should contain the title of the data set, the publisher, the place of publication, the date of the volume, the data entry number (as opposed to the data value), and the name of the figure or other identifying information. The page number can be included in the citation if page numbers are used in the index of the data set.

References to data retrieved from a stand-alone database should cite the source as a computer program (for example, MDL CrossFire Commander, see p 323 f) or as an online reference book (for example, the Kirk-Othmer Encyclopedia of Chemical Technology, see p 305 f), with the data entry number or other identifying information included at the end of the citation. Data retrieved from an Internet-based database should cite the source as a Web site (see pp 316 ff). If the data retrieved are calculated data, also cite the software used for calculation (for example, ACD/Labs).
Material Safety Data Sheets

Material Safety Data Sheets (MSDSs) are published by the company that manufactures the material covered on the sheet. Citations should include the title of the data sheet, which is the name of the material; the MSDS number; the manufacturing company; the location of the company; and the date on which the document was released. If the online version was used, the designation “Online” is included in brackets after the MSDS number, and the URL and date accessed are included at the end of the citation.

RECOMMENDED FORMATS

Title; MSDS Number; Manufacturing Company: Location of Company, Date.

Title; MSDS Number [Online]; Manufacturing Company: Location of Company, Date. URL (accessed Month Day, Year).


Unpublished Materials

Material in any stage preceding actual publication falls under this general classification, as do personal communications and work not destined for publication.

RECOMMENDED FORMAT FOR MATERIAL INTENDED FOR PUBLICATION

Author 1; Author 2; etc. Title of Unpublished Work. Journal Abbreviation, phrase indicating stage of publication.

Various phrases indicating the stage of publication are acceptable in these references.

➤ For material accepted for publication, use the phrase “in press”.


➤ For material intended for publication but not yet accepted, use “unpublished work”, “submitted for publication”, or “to be submitted for publication”.

Recommended format for printed data sets

Title; Publisher: Place of Publication, Date; Data Entry Number, Figure Title or other identifying information.


As Gordon G. Hammes says in Chapter 1 of this book,

Occasionally, the attribution of an idea or fact may be to a “private communication” of a colleague or fellow scientist. In such cases, permission must be obtained from the individual in question before the citation is made. Reference to unpublished material should be avoided if possible because it generally will not be available to interested readers.

**RECOMMENDED FORMAT FOR MATERIAL NOT INTENDED FOR PUBLICATION**

Author. Affiliation, City, State. Phrase describing the material, Year.


Messages sent by electronic mail are considered personal communications and are referred to as such.

**Electronic Sources**

Electronic media continue to develop rapidly in content, organization, and presentation of information. The conventions for citing electronic resources are evolving to reflect these changes, but the basic principles of citation remain the same: present enough documentation with enough clarity to establish the identity and authority of the source and direction for locating the reference. The guidelines stress consistency both in presentation of information and in reasons for exceptions.

To date, much of the material available in electronic media corresponds to and/or is modeled after the traditional print-based sources discussed earlier in this chapter and should be cited according to those guidelines as appropriate. However, given the transient nature of electronic sources, it is important to provide additional documentation about the format or online location and the date the source was accessed.

**Internet Sources**

Internet sources include online editions of traditional sources such as periodicals and books available through Web technology; new collective sites of information, including Internet-based databases using Web, file transfer protocol (FTP),
and Telnet technologies; and electronic mailing lists and mail messages that may or may not use Web interfaces. Each source has an electronic address; for sources using the World Wide Web, this address is called the uniform resource locator (URL). As Web interfaces and supporting technologies evolve, direct addresses of items will often change to reflect new structures. Changing addresses can disrupt access to information sources that may still be available but at new locations and in modified formats. This issue can be resolved locally through use of persistent URLs. A persistent URL remains constant, but the actual location of a source is tracked through a local database that can be updated without disrupting the URL.

Information sources can also be tracked globally through coordinated efforts such as the Digital Object Identifier (DOI) system. Information providers register their sources, which are assigned unique and persistent DOIs. Each DOI is similar to a barcode that manages a complex profile of multiple pieces, formats, locations, ownership rights, and interoperability features. The identity of and access to an electronic information source is maintained through its DOI regardless of changes in location, format, or publisher. The use of DOIs is spreading among publishers as an efficient system to manage journal articles and other types of intellectual property on the Web. Further information about the DOI system can be found at http://www.doi.org (accessed April 13, 2005).

CrossRef is an application of the DOI system that links online citations across publishers. The unique identification and persistent location information in the DOI is packaged into an open URL that publishers and libraries can use to link to subscribed full-text content from reference lists. These links appear with citations in the reference lists of online articles and databases from several participating publishers.

For the purposes of citation, reference style conventions continue to use the URL as the most direct route to the location of a source. DOIs are sometimes used by publishers in place of page numbers or article numbers and should be included in citations in this context.

> URLs can be long and complicated, and there are conventions for splitting an address between multiple lines; see Chapter 10 (pp 156–157) for guidelines on breaking URLs and e-mail addresses.

**Online Periodicals**
There are several types of periodicals online, including those based on print editions, electronic copies retrieved from databases, articles released online in advance of a full print issue, periodicals published only in electronic format, and article preprints posted in preprint servers. The reference styles for periodicals apply, with additional information concerning online location and accession date assigned as needed. As for print periodicals, article titles are desirable but not included in all ACS publications; check the publication itself.
RECOMMENDED FORMAT FOR ONLINE PERIODICALS
BASED ON PRINT EDITIONS

Author 1; Author 2; Author 3; etc. Title of Article. *Journal Abbreviation* [Online]* Year, Volume*, Inclusive pagination or other identifying information. URL (accessed Month Day, Year).

Currently, the majority of the articles retrieved from online publications are based on corresponding print versions. For these articles, the basic periodical reference style is used, but if the article has been viewed only in its electronic form, the designation “Online” is included in brackets after the journal abbreviation.


RECOMMENDED FORMATS FOR ELECTRONIC COPIES OF ARTICLES
RETRIEVED FROM A DATABASE PROVIDER

Author 1; Author 2; Author 3; etc. Title of Article. *Journal Abbreviation* [Online]* Year, Volume*, Article Number or other identifying information. Database Provider. URL of top page (accessed Month Day, Year).

Author 1; Author 2; Author 3; etc. Title of Article. *Title of Periodical* [Online], Complete Date, Pagination. Database Provider. URL of top page (accessed Month Day, Year).

Electronic copies of periodicals, nonscientific magazines, or newspapers retrieved from subscription database services often provide only the original text but not the original formatting or the figures. For online articles provided as content in a subscription database, use the reference style for periodicals or nonscientific magazines as appropriate, and include the name of the database provider, the URL of the top page, and the date accessed.


RECOMMENDED FORMAT FOR ARTICLES PUBLISHED ONLINE
IN ADVANCE OF PRINT ISSUES

Author 1; Author 2; Author 3; etc. Title of Article. *Journal Abbreviation* [Online early access]. DOI or other identifying information. Published Online: Month Day, Year. URL (accessed Month Day, Year).

Often, articles are ready for publication in advance of a full issue of a periodical. Several publishers offer these articles online up to weeks in advance of the print issue. They are identical to the corresponding print articles except that page numbers are often not yet available. Publishers market this service under different names; the ACS Publications Division labels them As Soon As Publishable (ASAP). For citation purposes, use the designation “Online early access” in brackets after the journal abbreviation in place of the publisher-specific term.
Also include the DOI or other identifying information, the online publication date, the URL, and the date accessed.


**RECOMMENDED FORMAT FOR PERIODICALS PUBLISHED ONLY IN ELECTRONIC FORMAT**

Author 1; Author 2; Author 3; etc. Title of Article. *Journal Abbreviation* [Online] *Year*, *Volume*, Article Number or other identifying information. URL (accessed Month Day, Year).

A periodical published only in electronic format may include additional electronic features, data, or commentaries. Use the reference style for periodicals, and include the direct URL of the article as well as the date accessed. Volume and page numbers are often not relevant. If they are not used, include the article number, DOI, or other identifying information.


**RECOMMENDED FORMAT FOR ARTICLES RETRIEVED FROM PREPRINT SERVERS**

Author 1; Author 2; Author 3; etc. Title of Article. Year, Article Number. Name of Repository. URL (accessed Month Day, Year).


**Online Books**

Books published online generally correspond to printed versions, and the reference styles are similar. Online location and access date should always be included when citing online books. Reference works published online are often updated with new content, and the dates on which sections were posted or updated should also be included.

**RECOMMENDED FORMAT FOR ONLINE BOOKS WITHOUT EDITORS**

Author 1; Author 2; Author 3; etc. *Book Title* [Online]; Series Information (if any); Publisher: Place of Publication, Year; Volume Number, Pagination. URL (accessed Month Day, Year).

**RECOMMENDED FORMAT FOR ONLINE BOOKS WITH EDITORS**

Author 1; Author 2; Author 3; etc. Chapter Title. In *Book Title* [Online]; Editor 1, Editor 2, etc., Eds.; Series Information (if any); Publisher: Place of Publication, Year; Volume Number, Pagination. URL (accessed Month Day, Year).


**RECOMMENDED FORMAT FOR ONLINE ENCYCLOPEDIAS**

Article Title. *Encyclopedia Title*, edition [Online]; Publisher, Posted Online Posting Date. URL (accessed Month Day, Year).


**Web Sites**

Aside from online periodicals and books, general Web sites containing a wide variety of information might need to be cited. Some sites are accessible by anyone, but many are accessible only by subscription. Reference styles for FTP and Telnet sites are similar to those for Web sites. Specific examples are given here for general Web sites and databases, stand-alone documents, unpublished conference proceedings, and electronic theses.

**RECOMMENDED FORMAT FOR GENERAL WEB SITES**

Author (if any). Title of Site. URL (accessed Month Day, Year), other identifying information (if any).

Use the title found on the Web site itself; add the words “Home Page” for clarification when needed. Data retrieved from Internet-based databases should include a data entry number. Stand-alone databases should be cited as computer programs (see p 323).


RECOMMENDED FORMAT FOR DOCUMENTS RETRIEVED FROM INSTITUTIONAL OR AGENCY WEB SITES

Author 1; Author 2; Author 3; etc. Title of Document, Year. Title of Site. URL (accessed Month Day, Year).

If an article is contained within a large and complex Web site, such as that for a university or a government agency, the host organization and the relevant program or department should be identified before giving the direct URL of the article and accession date.


RECOMMENDED FORMAT FOR ONLINE UNPUBLISHED CONFERENCE PRESENTATIONS

Author 1; Author 2; etc. Title of Presentation. Presented at Conference Title [Online], Place, Date; Paper Number. Title of Site. URL (accessed Month Day, Year).

Works presented at conferences or meetings can be cited in several formats, as discussed earlier in this chapter. Generally, published abstracts or proceedings can be cited as online books or as online periodicals. Materials from oral presentations, posters, or demonstrations that do not contain publication information should be cited as follows.


RECOMMENDED FORMAT FOR ELECTRONIC THESIS

Author. Title of Thesis. Level of Thesis [Online], Degree-Granting University, Location of University, Date of Completion. URL (accessed Month Day, Year).

Electronic Lists and Newsgroups

RECOMMENDED FORMAT FOR ELECTRONIC LISTS AND NEWSGROUPS

Mailing List or Newsgroup Name, other information, electronic address (accessed Month Day, Year).

Chemical Information List Server, CHMINF-L@iubvm.ucs.indiana.edu (accessed Oct 13, 2004).

Computational Chemistry List, solvent discussion in archived messages of September 2003, chemistry@ccl.net (accessed Nov 10, 2004).

Molecular Diversity for Basic Research & Drug Discovery, mol-diversity@listserv.arizona.edu (accessed Nov 10, 2004).

Electronic Mail Messages

Whether the message was personal and sent only to you or whether it was posted in a newsgroup, it is not published. E-mail messages should be cited the same as any other personal communication. Include the year and the professional affiliation of the author.

RECOMMENDED FORMAT FOR ELECTRONIC MAIL MESSAGES

Author. Affiliation, City, State. Personal communication, Year.

Solla, L. R. Cornell University, Ithaca, NY. Personal communication, 2005.

CD-ROMs and DVDs

The reference style for information published in CD-ROM or DVD format follows that for periodicals and books as appropriate, and the designation “CD-ROM” or “DVD” is included in brackets.

RECOMMENDED FORMAT FOR CD-ROM AND DVD PERIODICALS

Author 1; Author 2; Author 3; etc. Title of Article. Journal Abbreviation [CD-ROM or DVD] Year, Volume, pagination or other identifying information.


RECOMMENDED FORMATS FOR CD-ROM AND DVD BOOKS

Author 1; Author 2; etc. Chapter Title. In Book Title, Edition Number [CD-ROM or DVD]; Editor 1, Editor 2, etc., Eds.; Publisher: Place of Publication, Year; Volume Number.

Author 1; Author 2; etc. Chapter Title. Book Title, Edition Number [CD-ROM or DVD]; Publisher: Place of Publication, Year; Volume Number.


Many books in CD-ROM or DVD format are reference works, so they have no authors, editors, or chapter titles.


**RECOMMENDED FORMAT FOR CONFERENCE PROCEEDINGS ON CD-ROM OR DVD**

Author 1; Author 2; etc. Title of Presentation. In *Title of Conference*, Location of Meeting, Date of Meeting [CD-ROM or DVD]; Publisher: Place of Publication, Year; other identifying information.


**Computer Programs**

References to computer programs must be treated on a case-by-case basis. Five common presentations of computer programs are possible:

1. book format, with the name of the program as the title
2. technical report format
3. *CASSI* format
4. free style, as a simple listing of program title and author of program
5. thesis style

**Book Format**

**RECOMMENDED FORMAT**

Author 1; Author 2; etc. *Program Title*, version or edition; Publisher: Place of Publication, Year.

The recommended format is the same as that for a book citation, except that there are no chapters or pages. The name of the computer program, with any descriptors, is considered the title and is set in italic type. If you wish to include additional information about a program that is important for the reader to know, you may add it at the end of the reference with or without parentheses or append it to the title in parentheses before the semicolon.


RECOMMENDED FORMAT FOR COMMERCIAL SOFTWARE AND DATABASES

*Program Title*, version or edition; comments; Publisher: Place of Publication, Year.

References to data should include the data entry number or other identifying information at the end of the citation. The date of access can also be included if the database is updated frequently. If the data retrieved are calculated data, also cite the software used for the calculation (for example, ACD/Labs).

*Mathematica*, version 5.1; software for technical computation; Wolfram Research: Champaign, IL 2004.

*MDL CrossFire Commander*, version 7; Elsevier MDL: San Leandro, CA, 2004; BRN 635994.


Technical Report Format

RECOMMENDED FORMAT

Author. *Title of Report*; Technical Report Number; Publisher: Place of Publication, Year; Pagination (if any).

In a citation to a computer program as a technical report, a report or technical report number is included. As with book format, the name of the computer program is considered the title of the technical report.


CASSI Format

Because of the broad base from which *Chemical Abstracts* indexes work, computer programs, in the form of technical reports, may be referenced. In such cases, CASSI format would be appropriate.


Free Style

When only minimal information (e.g., author and program name) is available, present the information as simply as possible.
Programs used in this study included local modifications of Jacobson’s ALLS, Zalkins’s FORDAP, Busing and Levy’s ORFEE, and Johnson’s ORTEP2.

Lozos, G.; Hoffman, B.; Franz, C. SIMI4A, Chemistry Department, Northwestern University.

**Thesis Style**


**Collating References**

Collate all references at the end of the manuscript in numerical order if cited by number and in alphabetical order if cited by author. Do not include items in the reference list that are not cited in the manuscript. Check the publication for which you are writing. Some publications do not allow multiple references to be listed as one numbered entry; they prefer that each numbered entry include only one unique reference.

To collate references according to the author–date style, use the following format.

1. Alphabetize in order of the first authors’ surnames.

2. When the same first author is common to multiple references,
   - Group the single-author references first. List them chronologically. To distinguish among references having the same year, add a lowercase letter (a, b, c, etc.) to the year.
   - Group the two-author references next. List them chronologically. To distinguish among references having the same year, add a lowercase letter (a, b, c, etc.) to the year.
   - Group all multiple-author (three or more) references last. List them chronologically. To distinguish among references having the same year, add a lowercase letter (a, b, c, etc.) to the year.


Do not use the Latin terms ibid. (in the same place) or idem (the same) because the actual reference source cannot be searched on electronic databases.

**Reference/Citation Managers**

Software programs are available to assist with the process of collecting and collating references. With such programs, researchers can create personal electronic collections or libraries of references and tailor the formatting to any number of uses and publishing guidelines. Citations are parsed into searchable databases of component fields, and formatting templates draw on the data to produce reference lists in a variety of reference styles. The process is further enhanced by filters designed to correctly interpret the variety of incoming reference formats. Filters, fields, and templates are customizable to accommodate additional sources and styles.

Additional features have been developed to improve the convenience of these tools, including connection scripts for hundreds of public-access and subscription-based bibliographic databases and increased variety of field types to accommodate figures, cross-linking, personal annotation, etc. Plug-ins are available for word-processing packages to format citations within the text, reference lists, and lists of figures as authors write. There are also networking options for cooperative reference building and linking to full-text versions of references.

Researchers can search literature databases either directly or through a reference manager interface; import text, images, and figures from journal articles, Web sites, and other reference managers; arrange reference lists in numerous collections or libraries; search and retrieve records by any field; format footnotes, endnotes, and stand-alone bibliographies; share and co-edit these lists with colleagues; and export citations in hundreds of publication-specific styles in several languages. These software packages assist the research process from initial literature searching to writing and editing final publications.

Leading reference management programs include EndNote, Reference Manager, ProCite, RefWorks, and Biblioscape. EndNote, Reference Manager, and
ProCite are currently all owned by Thomson Scientific and are available as stand-alone software packages for both Windows and Macintosh platforms. RefWorks is a Web-based program with individual accounts that can be accessed across platforms from any point of Internet access. Biblioscape is available in a variety of stand-alone and Web-based options. For the most part, these programs cover the gamut of research disciplines and are fairly well populated with filters and templates specific to the chemistry literature. Reviews of these and other bibliographic management software tools are regularly available in the library literature.

The Thomson Scientific products were developed independently and still retain distinctive characteristics in their functionality. EndNote focuses on the reference input and output needs of the individual researcher, with hundreds of connection scripts and filters and more than 1000 citation style templates. EndNote is updated regularly and has a growing number of enhanced features available. Reference Manager has traditionally targeted collaborative reference sharing between colleagues, with networking options that allow multiple users to work on the same reference list for a project. Some of these features are now becoming available in EndNote as well. Reference Manager is only available for the Windows platform. ProCite has focused on managing reference collections with larger numbers of fields and reference types and more advanced grouping and searching techniques. ProCite has not been updated since version 5 in 2001.

RefWorks is published by RefWorks.com and emphasizes the convenience and collaborative nature of Web-based software. The program and updates are provided on the RefWorks server, and users’ bibliographic data are stored there as well. Multiuser accounts are available for collaborative work. The options for filters, fields, reference types, and templates are less developed in RefWorks than in the other tools discussed here and do not include filters or templates for ACS journal styles.

Biblioscape is published by CG Information, founded by scientists specifically to manage scientific and electronic information. Biblioscape is a suite of products with different sets of features designed for a variety of users, including undergraduate and graduate students, researchers, and librarians. Options include Web access, intranet, and freeware editions. More than 1000 output styles are available, including the ACS journal styles.
APPENDIX 14-1

CASSI Abbreviations for the 1000+ Most Commonly Cited Journals

This appendix lists the Chemical Abstracts Service Source Index, or CASSI, abbreviations for more than 1000 of the most commonly cited journals. Note that some journals of the same name are published in more than one city. Authors should check the journal name carefully and include the city to prevent misunderstanding.

ACS Symp. Ser.
Acta Hortic.
Acta Mater.
Acta Phys. Pol., B
Adv. Mater. (Weinheim, Ger.)
Adv. Sci. Technol. (Faenza, Italy)
Adv. Space Res.
AICHE J.
AIDS (London, U.K.)
AIDS Res. Hum. Retroviruses
AIP Conf. Proc.
Aliment. Pharmacol. Ther.
Am. Heart J.
Am. J. Cardiol.

Appl. Catal., A
Appl. Catal., B
Appl. Geochem.
Appl. Spectrosc.
Aquaculture
Aquat. Toxicol.
Arch. Biochem. Biophys.
Arch. Environ. Contam. Toxicol.
Arch. Pharmacal Res.
Arch. Virol.
ARKIVOC (Gainesville, FL, U.S.)
Arthritis Rheum.
Asian J. Chem.
Astron. J.
Astrophys. J.
Atherosclerosis (Amsterdam, Neth.)
Atmos. Chem. Phys.
Atmos. Environ.
Bandaoti Xuebao
Behav. Brain Res.
Biochem. Eng. J.
Biochem. J.
Biochem. Pharmacol.
Biochem. Soc. Trans.
Biochem. Syst. Ecol.
Biochemistry
Biochemistry (Moscow, Russ. Fed.)
Biochim. Biophys. Acta
Bioconjugate Chem.
Bioinformatics
Biol. Chem.
Biol. Psychiatry
Biol. Reprod.
Biomacromolecules
Biomaterials
Biophys. Chem.
Biophys. J.
Biopolymers
Biosci., Biotechnol., Biochem.
Biosens. Bioelectr.
BioTechniques
Biotechnol. Prog.
Blood
BMC Bioinf.
Bone (San Diego, CA, U.S.)
Bone Marrow Transplant.
Br. J. Anaesth.
Br. J. Cancer
Br. J. Haematol.
Br. J. Pharmacol.
Brain Res.
Breast Cancer Res. Treat.
Bull. Environ. Contam. Toxicol.
Bunseki Kagaku
C. R. Chim.
Cailiao Kexue Yu Gongcheng Xuebao
Cancer (New York, NY, U.S.)
Cancer Biol. Ther.
Cancer Cell
Cancer Chemother. Pharmacol.
Cancer Epidemiol., Biomarkers Prev.
Cancer Lett. (Amsterdam, Neth.)
Cancer Res.
Cancer Sci.
Carbon
Carbohydr. Polym.
Carbohydr. Res.
Carcinogenesis
Catal. Today
Cell (Cambridge, MA, U.S.)
Cell Biol. Int.
Cell Cycle
Cell Death Differ.
Cell. Signalling
Cem. Concr. Compos.
Ceram. Int.
Ceram. Trans.
Cereal Chem.
Chem. Biol.
Chem. Eng. J. (Amsterdam, Neth.)
Chem. Eng. News
Chem.—Eur. J.
Chem. Geol.
Chem. Lett.
Chem. Mater.
Chem. Phys.
Chem. Rev. (Washington, DC, U.S.)
Chem. Sens.
ChemBioChem
Chemosphere
ChemPhysChem
Chest
Chin. Chem. Lett.
Chin. Med. J. (Beijing, China, Engl. Ed.)
Chromatographia
Circ. Res.
Circulation
Clin. Exp. Allergy
Colloid Polym. Sci.
Colloids Surf., A
Colloids Surf., B
Combust. Flame
Integr. Physiol.
Comp. Biochem. Physiol., Part B:
Biochem. Mol. Biol.
Compos. Sci. Technol.
Corros. Sci.
Crit. Care Med.
Cuihua Xuebao
Curr. Sci.
Cytogenet. Genome Res.
Cytokine+
Dalton Trans.
Desalination
Dev. Biol. (San Diego, CA, U.S.)
Dev. Brain Res.
Dev. Cell
Dev. Dyn.
Development (Cambridge, U.K.)
Di-San Junyi Daxue Xuebao
Diabetes
Diabetologia
Diamond Relat. Mater.
Dianchi
Dianyuan Jishu
Dier Junyi Daxue Xuebao
Diffus. Defect Data, Pt. B
Dig. Dis. Sci.
Disi Junyi Daxue Xuebao
Diyi Junyi Daxue Xuebao
DNA Repair
Dokl. Earth Sci.
Drug Metab. Dispos.
Dyes Pigm.
EAAP Publ.
Earth Planet. Sci. Lett.
Ecotoxicol. Environ. Saf.
Electroanalysis
Electrochemistry (Tokyo, Jpn.)
Electrochim. Acta
Electron. Lett.
Electrophoresis
EMBO J.
EMBO Rep.
Endocrinology
Energy Fuels
Environ. Health Perspect.
Environ. Technol.
Environ. Toxicol. Chem.
Enzyme Microb. Technol.
Eukaryotic Cell
Eur. J. Cancer
Eur. Phys. J. A
Eur. Phys. J. D
Eur. Space Agency, [Spec. Publ.] SP
Europhys. Lett.
Exp. Cell Res.
Exp. Eye Res.
Exp. Gerontol.
Exp. Neurol.
Expert Opin. Invest. Drugs
Expert Opin. Pharmacother.
Farmaco
FASEB J.
FEBS Lett.
FEMS Microbiol. Lett.
Fenxi Huaxue
Fenxi Kexue Xuebao
Fenxi Shiyanshi
Ferroelectrics
Fish Physiol. Biochem.
Fiz. Khim. Tverd. Tila
Fluid Phase Equilib.
Food Addit. Contam.
Food Chem.
Food Chem. Toxicol.
Food Hydrocolloids
Forensic Sci. Int.
Free Radical Res.
Front. Biosci.
Fuel
Fusion Energy
Fusion Eng. Des.
Gangtie
Gaodeng Xuexiao Huaxue Xuebao
Gaofenzi Cailiao Kexue Yu Gongcheng
Gaofenzi Xuebao
Gaoneng Wuli Yu Hewuli
Gaoxiao Huaxue Gongcheng Xuebao
Gastroenterology
Gendai Iryo
Gene
Gene Expression Patterns
Gene Ther.
Genes Dev.
Genetics
Genome Res.
Genomics
Gongcheng Suliao Yingyong
Gongneng Cailiao
Gongye Cuihua
Green Chem.
Guangpu Shiyanshi
Guangpuxue Yu Guangpu Fenxi
Guangzi Xuebao
Guisuan Yan Xuebao
Gut
Gynecol. Oncol.
Haematologica
Handb. Exp. Pharmacol.
Han’guk Hwankyong Uisaeng Hakhoechi
Han’guk Sikp’um Yongyang Kwahak
Hoechi
Hecheng Huaxue (1000)
Hecheng Xiangjiao Gongye
Hepatol.ogy (Philadelphia, PA, U.S.)
Heterocycles
Horm. Metab. Res.
Huagong Shikan
Huagong Xuebaol (Chin. Ed.)
Huanjing Kexue Xuebao
Huanjing Wuran Zhili Jishu Yu Shebei
Huaxue Tongbao
Huaxue Xuebaol
Huaxue Yanjiu Yu Yingyong
Hum. Mol. Genet.
Hum. Mutat.
Hum. Pathol.
Hum. Reprod.
Hydrobiologia
Hyomen Gijutsu
Hyperfine Interact.
Hypertension
IEEE Trans. Electron Devices
Igaku no Ayumi
Immunology
Indian J. Environ. Prot.
Indian J. Pharm. Sci.
Infect. Immun.
Inflammation Res.
Inorg. Chem.
Inorg. Mater.
Insect Biochem. Mol. Biol.
Int. Conf. Thermoelectr.
Int. Congr. Ser.
Int. DATA Ser., Sel. Data Mixtures, Ser. A
Int. Immunol.
Int. Immunopharmacol.
Int. J. Antimicrob. Agents
Int. J. Cancer
Int. J. Food Microbiol.
Int. J. Heat Mass Transfer
Int. J. Hydrogen Energy
Int. J. Mass Spectrom.
Int. J. Mod. Phys. B
Int. J. Nanosci.
Int. J. Oncol.
Int. J. Parasitol.
Int. J. Pharm.
Int. J. Quantum Chem.
Integr. Ferroelectr.
Intermetallics
IP.com J.
ISIJ Int.
J. Alloys Compd.
J. Am. Chem. Soc.
J. Am. Coll. Cardiol.
J. Am. Oil Chem. Soc.
J. Am. Soc. Nephrol.
J. Anal. Appl. Pyrolysis
J. Anim. Sci. (Savoy, IL, U.S.)
J. AOAC Int.
J. Appl. Phys.
J. Appl. Physiol.
J. Appl. Spectrosc.
J. Bacteriol.
J. Biochem. (Tokyo, Jpn.)
J. Biol. Chem.
J. Biomol. NMR
J. Biosci. Bioeng.
J. Biotechnol.
J. Bone Miner. Res.
J. Catal.
J. Cell Physiol.
J. Cell Sci.
J. Chem. Eng. Data
J. Chin. Chem. Soc. (Taipei, Taiwan)
J. Chromatogr., A
J. Colloid Interface Sci.
J. Comp. Neurol.
J. Controlled Release
J. Coord. Chem.
J. Cryst. Growth
J. Dairy Sci.
J. Electroanal. Chem.
J. Endocrinol.
J. Environ. Eng. (Reston, VA, U.S.)
J. Environ. Monit.
J. Environ. Qual.
J. Environ. Radioact.
J. Essent. Oil Res.
J. Exp. Biol.
J. Exp. Bot.
J. Exp. Med.
J. Fluorine Chem.
J. Food Prot.
J. Food Sci.
J. Geophys. Res., [Atmos.]
J. Hazard. Mater.
J. Hepatol.
J. Heterocycl. Chem.
J. Histocom. Cytochem.
J. Hypertens.
J. Immunol.
J. Immunol. Methods
J. Indian Chem. Soc.
J. Infect. Dis.
J. Korean Ceram. Soc.
J. Leukocyte Biol.
J. Lipid Res.
J. Lumin.
J. Mass Spectrom.
J. Mater. Chem.
J. Mater. Res.
J. Mater. Sci.
J. Mater. Sci. Technol. (Shenyang, China)
J. Med. Chem.
J. Membr. Sci.
J. Microbiol. Methods
J. Mol. Biol.
J. Mol. Liq.
J. Mol. Spectrosc.
J. Mol. Struct.
J. Nat. Prod.
J. Neurochem.
J. Neuroimmunol.
J. Neurophysiol.
J. Neurosci.
J. Non-Cryst. Solids
J. Nucl. Mater.
J. Nutr.
J. Pathol.
J. Pharm. Pharmacol.
J. Pharm. Sci.
J. Pharmacol. Sci. (Tokyo, Jpn.)
J. Photochem. Photobiol., A
J. Phys. Chem. A
J. Phys. Chem. B
J. Phys. Chem. Solids
J. Phys.: Condens. Matter
J. Phys. IV
J. Plant Physiol.
J. Power Sources
J. Quant. Spectrosc. Radiat. Transfer
J. Radioanal. Nucl. Chem.
J. Raman Spectrosc.
J. Rheumatol.
J. Thromb. Haemostasis
J. Urol. (Hagerstown, MD, U.S.)
J. Vac. Sci. Technol., A
J. Virol.
J. Virol. Methods
JAERI—Conf
JETP Lett.
Jiegou Huaxue
Jikken Igaku
Jingxi Huagong
Jingxi Huagong Zhongjianti
Jinshu Xuebao
Jisuanji Yu Yinglyong Huaxue
Jixie Gongcheng Cailiao
Jpn. J. Appl. Phys., Part 1
Jpn. J. Appl. Phys., Part 2
Kagaku to Kogyo (Tokyo, Jpn.)
Kagaku to Kyoiku
Kagaku to Seibutsu
KEK Proc.
Key Eng. Mater.
Kidney Int.
Kogyo Zairyo
Kongop Hwahak
Lab. Invest.
Lancet
Langmuir
Leuk. Lymphoma
Leuk. Res.
Leukemia
Life Sci.
Low Temp. Phys.
Lung Biol. Health Dis.
Macromol. Symp.
Macromolecules
Mater. Lett.
Mater. Sci. Eng., A
Mater. Sci. Eng., B
Mater. Sci. Eng., C
Mater. Sci. Forum
Mater. Trans.
Meat Sci.
Mech. Dev.
Med. Hypotheses
Meded.—Fac. Landbouwkld. Toegepaste Biol. Wet. (Univ. Gent)
Metab., Clin. Exp.
Metall. Mater. Trans. A
Methods Enzymol.
Methods Mol. Biol. (Totowa, NJ, U.S.)
Methods Mol. Med.
Microbes Infect.
Microbiology (Reading, U.K.)
Microchim. Acta
Microelectron. Eng.
Microelectron. Reliab.
Microporous Mesoporous Mater.
Miner. Eng.
Mod. Phys. Lett. A
Mol. Biochem. Parasitol.
Philos. Mag.
Phosphorus, Sulfur Silicon Relat. Elem.
Phys. At. Nucl.
Phys. Fluids
Phys. Lett. A
Phys. Lett. B
Phys. Plasmas
Phys. Rev. D: Part. Fields
Phys.
Phys. Solid State
Phys. Status Solidi A
Phys. Status Solidi B
Phys. Status Solidi C
Physica B (Amsterdam, Neth.)
Physica C (Amsterdam, Neth.)
Physica E (Amsterdam, Neth.)
Physiol. Behav.
Physiol. Genomics
Physiol. Plant.
Phytochemistry (Elsevier)
Planta
Plant Cell
Plant Cell Physiol.
Plant J.
Plant Mol. Biol.
Plant Physiol.
Plant Sci. (Amsterdam, Neth.)
Plant Soil
Planta Med.
Plasma Phys. Controlled Fusion
Plast. Massy
Polyhedron
Polym. Int.
Polym. J. (Tokyo, Jpn.)
Polym. Chem.)
Polymer
Poult. Sci.
Powder Technol.
Poverkhnost
Pramana
Chem.
Proc.—Annu. Conf., Am. Water Works
Assoc.
Prostaglandins, Leukotrienes Essent. Fatty
Acids
Prostate (New York, NY, U.S.)
Protein Expression Purif.
Protein Sci.
Proteomics
Psychopharmacology (Berlin, Ger.)
Pure Appl. Chem.
Quim. Nova
Ranliao Huaxue Xuebao
Recents Prog. Genie Procedes
Regul. Pept.
Rengong Jingti Xuebao
Reproduction (Bristol, U.K.)
Res. Discl.
Rev. Chim. (Bucharest, Rom.)
RILEM Proc.
Rinsho Men’eki
RNA
Russ. J. Appl. Chem.
Russ. J. Electrochem.
Russ. J. Genet.
Saibo Kogaku
Sci. Total Environ.
Science (Washington, DC, U.S.)
Scr. Mater.
Sekitan Kagaku Kaigi Happyo Ronbunshu
Semiconductors
Sens. Actuators, A
Sens. Actuators, B
Sepu
Shandong Daxue Xuebao, Yixueban
Shengwu Yixue Gongchengxue Zazhi
Shijie Huaren Xiaohua Zazhi
Shipin Kexue (Beijing, China)
Shiyou Huagong
Shiyou Lianzhi Yu Huagong
Shock
Soil Sci. Soc. Am. J.
Solid State Commun.
Solid-State Electron.
Solid State Ionics
Spectrochim. Acta, Part A
Spectrochim. Acta, Part B
Steroids
Stroke
Structure (Cambridge, MA, U.S.)
Surf. Interface Anal.
Surf. Sci.
Symp.—Int. Astron. Union
Synlett
Synth. Met.
Synthesis
Talanta
Tetrahedron
Tetrahedron: Asymmetry
Tetrahedron Lett.
Text. Res. J.
Tezhong Zhuzao Ji Youse Hejin
THEOCHEM
Theriogenology
Thermochim. Acta
Thin Solid Films
Thromb. Haemostasis
Thromb. Res.
Tissue Antigens
Tissue Eng.
Tokyo Daigaku Genshiryoku Kenkyu Sogo
Senta Shinpojumu
Top. Catal.
Toxicol. Lett.
Toxicol. Sci.
Toxicology
Toxicon
Trans. Nonferrous Met. Soc. China
Transition Met. Chem. (Dordrecht, Neth.)
Transplant. Proc.
Transplantation
Trends Opt. Photonics
Tsvetn. Met. (Moscow, Russ. Fed.)
Vaccine
Vacuum
VDI—Ber.
Virology
Virus Res.
Water, Air, Soil Pollut.
Water Res.
Wear
World J. Gastroenterol.
Wuji Cailiao Xuebao
Wuji Huaxue Xuebao
Wuli Huaxue Xuebao
Wuli Xuebao
Xibao Yu Fenzi Mianyixue Zazhi
Xiyou Jinshu
Xiyou Jinshu Cailiao Yu Gongcheng
Yaoxue Xuebao
Yingyong Huaxue
Yingyong Shengtai Xuebao
Youji Huaxue
Z. Metallkd.
Z. Naturforsch., C: J. Biosci.
Zairyo
Zhengzhou Daxue Xuebao, Yixueban
Zhongcaoyao
Zhongguo Bingli Shengli Zazhi
Zhongguo Dongmai Yinghua Zazhi
Zhongguo Gonggong Weisheng
Zhongguo Jiguang
Zhongguo Jishui Paishui
Zhongguo Shenghua Yaowu Zazhi
Zhongguo Shengwu Gongcheng Zazhi
Zhongguo Shengwu Huaxue Yu Fenzi
Shengwu Xuebao
Zhongguo Shouyi Xuebao
Zhongguo Suliao
Zhongguo Xinyao Zazhi
Zhongguo Xitu Xuebao
Zhongguo Yaolixue Tongbao
Zhongguo Yaoxue Zazhi (Beijing, China)
Zhongguo Yiyao Gongye Zazhi
Zhongguo Yiyuan Yaoxue Zazhi
Zhongguo Youse Jinshu Xuebao
Zhonghua Yixue Yichuanxue Zazhi
Zhongliu Fangzhi Zazhi
APPENDIX 14-2

A Sample CASSI Entry


**AMERICAN CHEMICAL SOCIETY. JOURNAL. WASHINGTON, D. C.**

Doc. Supplier: CAS.

AAP; AB 1905+; ABSR; ARaS; ATVA; AU–M 1893–1918,1920–1926,1928+; AkU 1879–1906,1919+; ArU; ArU–M 1923+; AzTeS; AzU 1889+; C; CL; CLSU; CLSU–M 1895–1897,1905,1908+; CLU–M; CLU–P; CMenSR 1916+; CPT; CSf; CSt; CSt–L; CU; CU–A; CU–I 1920+; CU–M; CU–Riv 1907+; CU–RivA; CU–RivP; CU–S; CU–SB; [etc.]

In this example,

- *Journal of the American Chemical Society* is the complete publication title with its abbreviated form indicated by boldface type (*J. Am. Chem. Soc.*).
- **JACSAT** is the CODEN, a six-character, unique title abbreviation used to represent titles in manual or machine-based information systems. The CODEN source is the *International CODEN Directory*, administered by Chemical Abstracts Service. The sixth character of each CODEN is a computer-calculated check character that ensures the reliability of the CODEN in computer-based systems.
- **ISSN 0002–7863** is the International Standard Serial Number (ISSN), assigned by the Library of Congress.
- **Absorbed Am. Chem. J.** is a reference to former titles and to any variant forms of the selected title.
- **In English; English sum.** is the language of the publication, summaries, and tables of contents.
- **History: v1 1879+** is the history of the publication. Volume 1 began in 1879. The + following the year indicates that the publication is still in existence under that title.
- **w** means weekly. The frequency of publication could also be *a* for annually, *ba* for biennially (every two years), *bm* for bimonthly (every two months), *bw* for biweekly (every two weeks), *d* for daily, *m* for monthly, *q* for quarterly, *sa* for semiannually (two times per year), *sm* for semimonthly (two times per month), or *sw* for semiweekly (two times per week).
• **126 2004** is the volume–year correlation (i.e., the first volume number of that year, which is the most recent covered by that edition of *CASSI*; volume 126 was the first volume number of 2004).

• **ACS Journals or Maruzen** is the publisher or source address or abbreviation.

• **AMERICAN CHEMICAL SOCIETY. JOURNAL. WASHINGTON, D. C.** is the AACR entry. This is the abbreviated entry as catalogued according to the Anglo-Ameri-

• **Doc. Supplier: CAS** means that articles are available through the CAS Document Delivery Service.

• **AAP; AB 1905+; ABSR;** etc., is the library holdings information. Libraries are identified by their *National Union Catalog* symbols, and holdings are shown by inclusive years.
This chapter discusses methods of preparing and submitting the figures and other illustrations that accompany a scientific paper for publication. The past 10 years have seen a radical technological shift in the way figures are created by authors and handled by publishers. Whereas authors previously submitted figures that were camera-ready—that is, ready for the printer’s camera to photograph before making printing plates—today many authors create figures using computer software, and most publishers encourage electronic versions of figures. This chapter presents guidelines for working with figures using the computer tools currently in widespread use; it also includes recommendations regarding the use of color, fonts, and scanners, as well as good style for citing and captioning figures.

Technical requirements and certain style points differ from publisher to publisher and from journal to journal, so bear in mind that this chapter presents general guidelines. ACS journals have some specific requirements that may differ from the general guidelines presented here, and these are noted throughout the chapter. As always, before you finalize figures for your manuscript, you should consult your publisher’s guidelines for submitting artwork. For ACS journals, consult recent issues as well as the Guide, Notes, or Instructions for Authors that appear in each journal’s first issue of the year or at https://paragon.acs.org/paragon/index.jsp (see “Author Information”). For ACS books, consult the brochure “How To Prepare Your Manuscript for the ACS Symposium Series” or see “Info for Authors” at https://pubs.acs.org/books.
Box 15-1. Do I Need a Figure or a Table?

Do I want the basic point to be communicated at a glance?  
*Use a figure.*

Do I want the reader to see trends and relationships?  
*Use a figure.*

Do I want the reader to see exact numbers?  
*Use a table.*

Do I want to communicate a lot of information with words?  
*Use a table.*

When To Use Figures

A *figure* is an illustration used in scientific or scholarly publishing. Figures can be graphs of data, photographs, sketches, flow charts, and so on. Figures can play a major role in highlighting, clarifying, and summarizing data and results and can substantially increase the readers’ comprehension of the text by communicating visually. For example, line graphs show trends. Bar graphs compare magnitudes. Pie charts show relative portions of a whole. Photographs can provide absolute proof of findings. In general, figures should be used when the picture really is worth a thousand (or so) words.

However, figures can decrease a reader’s comprehension, and they can cause outright confusion if they are poorly rendered or cluttered, if they do little more than repeat data already presented in text, or, worse, if they present information at odds with the text. An excessive number of figures can dilute the value of any individual figure: when presented with too many figures, a reader may look carefully at none of them. Figures should not be used to present data that would be better presented in a table. See Box 15-1 and Chapter 16, “Tables.”

The cost of publishing figures has decreased substantially over the past two decades, partly because authors are able to prepare better quality figures (so the publisher does not have to) and partly because of the shift to electronic methods of Web and print publishing that are less cumbersome than earlier technologies, which required a high-quality, pristine paper original of all art. The cost of publishing color figures has also decreased substantially because most color photographs can now be provided in electronic form and no longer require expensive color separations before being put on a printing press. The cost of using color in Web publications is inconsequential (although color should still be used carefully to enhance your meaning, not just to grab attention). See Box 15-2.
Box 15-2. Do I Need To Use Color?

Do I need color to make the picture comprehensible to the reader?

*Color should be used only when it is essential to understand the chemical nature of the material in the picture. Otherwise the picture should be prepared in black and white.*

Do I need color in my line graph, bar graph, or pie chart?

*Color is rarely required in these figures. Lines with varying dash styles in line graphs and distinct grayscale shades in bar graphs or pie charts work as well.*

Do I need color to catch the reader’s eye?

*No.*

Do I need color to organize related information for the reader?

*No. Judicious use of fonts and careful placement of words and objects usually does just as well.*

How To Cite Figures

All figures must be “called out”, that is, mentioned or discussed by name and number in the text. (If you cannot find a graceful, logical place to put the callout, then you might consider deleting the figure.) Follow these guidelines in citing figures.

➤ Capitalize the word “Figure” when it is followed by the figure number.

➤ Number figures sequentially with arabic numerals in order of discussion in the text (Figure 1, Figure 2, etc.).

➤ Designate parts of a figure by using a combination of the arabic numeral and a sequence of consistent labels, usually (but not always) letters: Figure 1a, Figure 1b; Figure 1A, Figure 1B; Figure 1-I, Figure 1-II. Do not cite, for example, Figure 4 and Figure 4A.

**EXAMPLES OF FIGURE CALLOUTS IN TEXT**

The block copolymers may contain a small but detectable fraction of impurities, as shown in Figures 1 and 2.

Figures 3–5 show the production of acid-reactive substances in three different oils.

The deuterium-labeled substrate gave rise to the partial $^1$H NMR spectra shown in Figure 2a,b.
As seen in Figure 3b–d, the catalytic wave shows a small but distinct decrease upon addition of the nucleophile.

Parts a and b of Figure 4 illustrate that the voltammetric plateau current depends on the number of enzyme monolayers.

Curves c–e of Figure 5 were obtained for various methyl groups in the protein.

**Poor examples of figure callouts in text**

Figure 2c and Figure 2D show… *should read* Figure 2c,d shows…

Figure 3 and Figure 4 show… *should read* Figures 3 and 4 show…

Chemical structures and schemes should not be numbered as figures; they should be labeled according to separate sequences. See Chapter 17, Chemical Structures.

**How To Prepare Figures**

At one time, almost all publishers required that figures be submitted as camera-ready artwork. Today, most publishers accept, many encourage, and a few require that figures be submitted in electronic format. Most scientists store their data on computers and create their figures using computer software, and good-quality document scanners are in common use. Thus, the submission of electronic files is simpler than ever before and has the advantage of keeping original data and photographs in the author’s own hands. Satisfactory results in the final publication are not guaranteed, however, and the burden rests on authors to prepare figures to suit the requirements of the medium in which they will be published.

**Publication Medium**

The traditional method for publishing books, journals, and other documents is *by print publishing*, that is, the application of ink on paper. Newer avenues include publishing on the Internet, usually called *Web publishing*, as well as other formats that are viewed on a computer monitor, such as CD-ROMs. The requirements of ink-on-paper and pixels-on-screen publishing are quite different and may affect your choices regarding figure creation and final electronic format. For printed materials to be satisfactory, the figure files must have much detail and therefore must be prepared at a higher resolution, that is, a higher number of pixels per inch (ppi). Paper printers also use a scale called dots per inch or dpi, which you may need to use sometimes. Materials viewed on a computer monitor do not require the same level of detail but—on the Web especially—they must download quickly, so they are prepared at a low resolution. Only for printed materials is color significantly more expensive than black-and-white, so in print, color is used conservatively. Conversely, on a computer monitor, color costs nothing additional and is used widely.
Publishing with ACS: When preparing figures for ACS journals—which are published in print and on the Web—prepare your figures to the higher standard required for print. ACS routinely prepares the Web figures from files provided for the print figures.

Types of Figure Artwork

The two broad categories of figure artwork are line art and continuous-tone art. Line art consists of black markings on a white background, with no additional colors and no shades of gray (see Figure 15-1A). Line art contains lines, solid shapes, and type (letters or words). Examples of line art include line graphs, flow charts, and scatter plots. (Structures and schemes are usually line art as well; see Chapter 17.) Continuous-tone art (also called halftone art) contains shades of gray (or color) (see Figure 15-1B). Examples of continuous-tone art include photographs (whether black-and-white or color) and drawings or sketches with midtones.

In print publishing, line art is straightforwardly rendered by ink on paper. To print continuous-tone art, the shading must be converted into dots through a process called screening. The size and spacing of the dots produces the illusion of shading to the reader’s eye. Halftones do not reproduce type or fine lines well because screening distorts the edges of the letters and lines. On a computer monitor, all text and images are converted to uniformly sized pixels.

Until recently, publishers strongly encouraged authors to submit figures as line art, with halftones reserved for photographs. Currently available software and the prevalence of electronic file submission is bringing a third category of art into more common use. Grayscale line art is black-and-white art that contains gray shading alongside fine lines and type (see Figure 15-1C). Grayscale line art may be used for pie charts, bar graphs, and area graphs, where different sections are distinguished by different shades of gray.

A fourth category of art is a combination of a photograph with some type, or a combo (see Figure 15-1D). An example might be a photomicrograph with a unit-of-measure legend in one corner; another might be a photograph with callouts identifying parts of an image, such as a piece of equipment. If there is only a small amount of type (as in the first example), then a combo can be handled like other halftones. When there is more type (as in the second example), then a combo requires special handling, because screened type loses legibility very quickly.

Publishing with ACS: For ACS journals, line art should be created and saved at 1200 ppi. Grayscale art, including grayscale line art and combos, should be created and saved at 600 ppi. Halftones, whether black-and-white or color, should be created and saved at 300 ppi.
Figure 15-1. Examples of categories of figure art: (A) line art, (B) halftone or continuous-tone art, (C) grayscale line art, and (D) a combo.

Figure 15-1. Continued.
Use of Color

The use of color in figures depends partly on the medium and partly on a particular publisher’s preferences. As mentioned earlier, color can be used in Web publishing at virtually no cost, so the only restrictions have to do with scientific effectiveness and good taste. Color in print publishing adds to the cost, so before preparing figures in color, you should ascertain a publisher’s policies on color.

Publishing with ACS: ACS journals do not require authors to pay the cost of color illustrations. Authors who publish color figures in ACS books are asked to pay half the cost.

In publications, color is produced by one of three modes:

- Black-and-white, or B&W: For print publications, where only one color of ink (usually black) is used.
- Cyan–magenta–yellow–black, or CMYK (also called four-color): For print publications, where all shades of color are produced by layering screened dots of four standardized inks.
- Red–green–blue, or RGB: For Web publications and others viewed on computer monitors, where all shades of color are produced by overlapping red, green, and blue light.

Most publishers can switch electronically from CMYK to RGB, although it is always better to use the publisher’s preferred format. Switching from one of the color formats to B&W may produce unsatisfactory results, however. If the gray tones that result are hard to distinguish from each other, a figure that was intelligible in color can become meaningless in B&W. For this reason, it is always better to prepare art that will be reproduced in black and white as B&W.

Electronic File Formats

Many software packages are available today for drawing, scanning, and manipulating figures. When a figure is saved in a format that can be read or reopened only by the software that produced it, the file is called an application file. Examples include files with names that end with the suffix .cdx, which can be opened only in Cambridgesoft ChemDraw, or files with names that end in the suffix .psd, which can be opened only in Adobe Photoshop. Application files often pose problems in both Web and print publishing because the publisher (or reader) might not have the necessary software to open or view the file. Many publishers will not accept application files for figures.

There are a handful of file formats, however, that can be opened in many different software packages. Drawing and scanning programs generally provide the option of saving to one or more of these formats. For example, ChemDraw and
Photoshop will both export figures as TIFFs, a format frequently used for print publications. The most universally accepted of these formats are the following:

**For Print**
- Encapsulated PostScript, or EPS. PostScript is a programming language developed by Adobe to describe pages, graphics, and fonts; an EPS file is coded to be embedded in a large PostScript file.
- Tagged Image File Format, or TIFF. TIFFs describe an image by dividing it into a grid of pixels and assigning a value to each square. The quality of a TIFF image depends on its resolution (in ppi), that is, the size of the original grid.

**For Web**
- Graphics Interchange Format, or GIF. GIF is a pixel-based format like TIFF, except the resolution is preset at 72 ppi, which is appropriate for the Web but seldom acceptable for print.
- Joint Photographic Experts Group, or JPEG. JPEG is another pixel-based format like TIFF but capable of higher resolutions than GIFs. JPEGs, however, are actually compressed files, and they lose small amounts of digital information every time they are opened, recompressed, and saved, so JPEG images tend to degrade with repeated processing. Only “fresh”, high-quality JPEGs are suitable for print publication.

**For Print and Web**
Many publishers now accept properly created Portable Document Files, or PDFs. A PDF document is created when an application file produced by any of a number of software programs is “distilled”, using software such as Adobe’s Acrobat Distiller. The PDF document can be viewed on any platform using viewing software such as Adobe’s Acrobat Reader, regardless of whether the viewer has the original application software.

**Publishing with ACS:** For ACS journals, figure art that will be submitted in PDF format should be distilled using Adobe Acrobat Distiller’s “Press Quality” setting.

With so many different software packages and file formats, there is no single “right” way to prepare figures for publication. A few common paths are listed here:
- A line-art figure is drawn in an application such as Adobe Illustrator, Macromedia Freehand, or Corel Draw and exported as an EPS or a TIFF file.
- A B&W photograph is scanned with the scanner’s software and saved as a grayscale TIFF.
A color digital photograph cropped in Photoshop is saved as a 72 ppi RGB GIF file for the Web or a 300 ppi CMYK TIFF file for print.

Grayscale line art is drawn in an application, such as Illustrator or Freehand, and saved as an EPS file.

Table 15-1 lists image file formats commonly accepted by publishers and their suitability for different publishing media and types of artwork.

Several software packages that are in common use can produce satisfactory GIFs for Web publishing but do not export images in a form that is acceptable for the more rigorous requirements of print. Corel WordPerfect and Microsoft Word, Excel, and PowerPoint cannot save figures as valid PostScript files or export directly to TIFFs. Box 15-3 offers suggestions for preparing publishable figures in that program.

### Sizing Artwork

Always determine the size at which your figures will be printed and prepare the final electronic version to those dimensions. Consult guidelines from the publisher first. If there are no guidelines, use the following:

- For a Web publication, size your artwork so that it is visually appealing and all parts of the graphic are easily readable on your monitor at 100%.

---

Table 15-1. Image File Formats and Their Suitability by Publication Medium and Type of Figure

<table>
<thead>
<tr>
<th>File Format</th>
<th>Optimal ppi</th>
<th>Web</th>
<th>B&amp;W Printing</th>
<th>Color Printing</th>
<th>Photographic</th>
<th>Grayscale Line Art</th>
<th>Combos</th>
</tr>
</thead>
<tbody>
<tr>
<td>GIF</td>
<td>72</td>
<td>H</td>
<td>X</td>
<td>X</td>
<td>R</td>
<td>R</td>
<td>R</td>
</tr>
<tr>
<td>RGB JPEG</td>
<td>72</td>
<td>R</td>
<td>X</td>
<td>X</td>
<td>R</td>
<td>R</td>
<td>R</td>
</tr>
<tr>
<td>B&amp;W JPEG</td>
<td>300</td>
<td>X</td>
<td>R</td>
<td>X</td>
<td>X</td>
<td>R</td>
<td>R</td>
</tr>
<tr>
<td>CMYK JPEG</td>
<td>300</td>
<td>X</td>
<td>X</td>
<td>R</td>
<td>X</td>
<td>R</td>
<td>R</td>
</tr>
<tr>
<td>Bitmap TIFF</td>
<td>1200</td>
<td>X</td>
<td>H</td>
<td>X</td>
<td>H</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>Grayscale TIFF</td>
<td>600–1200</td>
<td>X</td>
<td>X</td>
<td>R</td>
<td>X</td>
<td>R</td>
<td>R</td>
</tr>
<tr>
<td>CMYK TIFF</td>
<td>300</td>
<td>X</td>
<td>X</td>
<td>H</td>
<td>X</td>
<td>H</td>
<td>R</td>
</tr>
<tr>
<td>EPS</td>
<td>N/A</td>
<td>X</td>
<td>R</td>
<td>H</td>
<td>H</td>
<td>X</td>
<td>H</td>
</tr>
</tbody>
</table>

*H indicates highly recommended; R indicates recommended; X indicates not recommended.

b The optimal number of pixels per inch (ppi) for art prepared to the size at which it will be published. It is always permissible to supply art with a higher ppi than what is listed here.

c EPS files are the best way to submit grayscale line art and combos, but the fonts used must be embedded or converted to outlines.
Box 15-3. Tips for Submitting Figures Created in Excel

Microsoft Excel and PowerPoint are widely used to create graphs and other figures, but they are unable to export to TIFF or any PostScript file format. Therefore, if figures prepared with these software programs are destined for print publication, they must be printed on paper first and then scanned. (It may also work to submit the figure as a PDF.) Moreover, the default settings of these programs will not produce satisfactory figures. The following tips help you get the best results from Excel.

- Do not use color to differentiate areas of the figure. Use black only for a color, and use gray tones to differentiate areas of the figure.
- Be sure that the weight of all lines is at least 0.5 point. Some lines in Excel default to 0.12 point, which is too thin for scanning. If the figure will be printed large and then reduced, calculate the width of lines accordingly (see the chart below).
- Be sure that the type and symbols also will scale down accordingly.
- It is better for tick marks to extend into the figure, rather than extend outside.
- Print the figure on clean, opaque, white paper, using a fresh ink or toner cartridge. Do not use a dot matrix printer. Set the laser or inkjet printer to a resolution of at least 600 ppi.
- Scan the figure to the correct size, and save it as a 600 ppi bitmap TIFF.

If your publisher requests the Excel application file, be sure that the source data are embedded (not linked) in the file you send.

Line width for a typical figure created in Excel, printed landscape on 8.5 × 11 in. paper, and destined to be printed at a width of 20 or 27 picas:

<table>
<thead>
<tr>
<th></th>
<th>20 picas (single-column journal)</th>
<th>27 picas (6 x 9 in. book)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Approximate reduction</td>
<td>38%</td>
<td>50%</td>
</tr>
<tr>
<td>Type size in Excel</td>
<td>14 pt</td>
<td>14 pt</td>
</tr>
<tr>
<td>Type size after reduction</td>
<td>5 pt</td>
<td>7 pt</td>
</tr>
<tr>
<td>Line width in Excel</td>
<td>1.5 pt</td>
<td>1 pt</td>
</tr>
<tr>
<td>Line width after reduction</td>
<td>0.5 pt</td>
<td>0.5 pt</td>
</tr>
</tbody>
</table>
For a printed publication, you can determine the column width and page length by measuring a sample copy of the journal or a similar book from the same publisher.

- For ACS journals, try to design figures to fit the width of one column. Table 15-2 gives the column widths and page lengths of many ACS publications.
- Do not put unnecessary frames or boxes around your figures.
- Remember that the length that you measure or take from Table 15-2 is the maximum space available for the figure plus captions or notes. Therefore, the art must be small enough to leave space for the caption.
- Finally, the width and depth of a figure should not exceed the needs of that figure. Be economical; do not waste space.

## Working with Line Art

If you are creating line-art figures with a computer program, save them in an appropriate format (see Table 15-1) or print them on white, high-quality, smooth, laser-printer paper and scan them. If line-art figures are being drawn by hand, use black ink on white, high-quality, smooth, opaque paper, and then scan them. Box 15-4 provides tips for successful scanning.

Here are some ways to improve the quality of the line-art figures you submit:

- Select software that will yield the best results for the line art you wish to create.
Box 15-4. Tips for Successful Scanning

- If possible, use a flatbed scanner, where the art rests flat on a glass surface and is scanned by a moving scanner’s eye, rather than a sheet-fed scanner, where the art is rolled past the scanner’s eye. Flatbed scanners are less likely to distort your figure.

- Use your scanner’s optical (that is, actual) resolution capability, not the interpolated (that is, calculated) one.

- Scan photographs at a minimum resolution of 300 ppi.

- Scan line art at a resolution of minimum 600 ppi, but 800, 1000, or 1200 ppi is even better. (Line art for ACS publications must be 1200 ppi.)

- If possible, determine the final size of your figure in print and calculate the percentage of expansion or reduction. Then scan the photograph at that percentage.

- If you are not sure about the final size, scan your photograph at a larger size (say, 150% with 300 ppi) or higher resolution (say, 100% with 450 ppi). Scan your line art at 150% with 600 ppi or at 100% with 1000 ppi. It is better to submit image files with too much information than too little.

- Do not adjust contrast or color according to what you see on your monitor. Instead, use the automatic adjustments that come with the scanning software or use the calibration curves that come with image-editing software, such as Photoshop.

- Do not apply any screening in the scanning or editing software, even if you know the figure will be screened before it is published. Let the publisher and the publisher’s printer determine the appropriate screening.

Create the line art to the exact size at which it will be published.

Keep line-art figures clear and simple. Keep words to a minimum. Lengthy explanations should go in the caption or a note accompanying the caption.

Scale the length, width, type, symbols, and lines of the art proportionally; keep the symbols, lines, and type at uniform density, or darkness.

- Make the lines at least 0.5 point wide and usually not more than 1.5 points wide.
Box 15-5. Type Size and Font

In publishing, type is measured in points; space is measured in picas. There are 72 points to an inch; there are 6 picas to an inch. The size of the type you are reading on this page is 10 points. The column is 28 picas wide, and the text page is 44 picas long.

You can use a pica ruler to measure space, but it is hard to find a type gauge for measuring type; you must compare it to known type sizes. For example, in 10 point type, no character actually is 10 points high.

The font (or typeface) is the style or design of the letters. There are literally hundreds of fonts, but plain, simple fonts such as Helvetica or Times Roman are best for scientific art.

Type also comes in different weights. Most of the type you are reading is lightface; **this is boldface type**. Type may be italic or roman. Generally, you should use lightface, roman type for figures.

This is 12 point Times Roman.

\[ ^{14}\text{C}_6\text{H}_6 \text{ shows subscripts and superscripts.} \]

This is 12 point Helvetica.

\[ ^{14}\text{C}_6\text{H}_6 \text{ shows subscripts and superscripts.} \]

This is 14 point Times Roman.

\[ ^{14}\text{C}_6\text{H}_6 \text{ shows subscripts and superscripts.} \]

This is 14 point Helvetica.

\[ ^{14}\text{C}_6\text{H}_6 \text{ shows subscripts and superscripts.} \]

- Select a type size of 7–10 points; for ACS journals, select a type size of 5–6 points.
- Make the symbols at least the size of a lowercase letter “oh” (about 2 mm) (see Box 15-5).
- Use a clear type font, preferably Helvetica or Times Roman (see Box 15-6).
- Disparities between the size of the type and the symbols make for illegible or unattractive art; if the type is the right size, the symbols will appear too small or too large, and vice versa. Likewise, the proportion between the overall size of the figure and the type and symbols should be appropriate (see Figure 15-2).

➤ Use simple, common symbols that would not be confused with each other and would be readily available in any publishing house, for example, \( \bigcirc, \bigotimes, \square, \blacksquare, \triangle, \Delta, \nabla, \nabla, \bigcirc, \bigotimes, \bigoplus, +, \times, \star, \text{ and } \bigstar. \) (Even if you provide a legend within the figure, you may wish to refer to the symbols in your text.)
Box 15-6. Tips Regarding Fonts

The fonts used to create some types of electronic figure files occasionally cause problems for publishers, in both print and Web publications. The problems can include character substitution, distorted spacing between letters, and copyright infringement.

The software behind a font is covered by copyright law. Whereas some copyright holders allow open access to their fonts, others exercise some sort of limit. Publishers respect the copyright on fonts and will not use a font without proper permission.

Only some electronic files embed font software in the files.

- GIFs, TIFFs, JPEGs, and other pixel-based files embed only the images of letters, not the font software itself, in their files. Type in these files can be erased, but it is not truly editable.
- EPS and PDF files must have font software fully embedded to be usable. Type in these files is fully editable.

TrueType is a font format designed by Microsoft for maximum legibility on a computer monitor, and it prints well on dot-matrix, inkjet, and laser printers. Microsoft permits free use of the fonts it provides (such as Times New Roman and Arial), but other companies that provide TrueType fonts may have use restrictions. TrueType fonts perform well in Web publishing, but they often pose technical problems in print publishing. TrueType fonts are fine for producing GIFs, TIFFs, and JPEGs, as well as PDFs intended for the Web.

PostScript is a font format designed for high-end graphic arts. These fonts are designed for maximum legibility on paper and for maximum compatibility with high-quality, high-output printing equipment. PostScript fonts are generally covered by copyright and have limitations on their use. They seldom pose technical problems in print publishing, but the copyright issues may limit their usefulness in Web publishing. PostScript fonts are best for EPS files and PDFs intended for print.

OpenType fonts are a relatively new format intended to combine the virtues of both TrueType and PostScript fonts.

STIX (scientific and technical information exchange) fonts were developed by a group of six scientific publishers to establish a comprehensive set of fonts that contains essentially every character that might be needed to publish a technical article in any scientific discipline. STIX fonts are available as a free download, under license, at www.stixfonts.org. A white paper by Tim Ingolsby on the STIX fonts project is available at www.aipservices.org/newsroom/white_papers/pdf/STIX-fonts.pdf.
Lines may be differentiated by the use of varying line styles, such as solid, dashed, dotted, and various weights (but never less than 0.5 point wide).

You may combine curves plotted on the same set of axes, but do not put more than five curves in one figure. (If you have more than five curves, consider splitting the figure into two parts or two separate figures.) Label all curves clearly. Leave sufficient space between curves; they should not overlap so much that they become indistinguishable.

Figure 15-2. (A) Example of a poorly rendered line graph, with lines that are too thin, a type font that is too ornate, and type and symbols that are sized disproportionally to the figure. (B) Example of the same line graph properly rendered.

Keep line-art figures compact; draw axes only long enough to define the contents. For example, if the highest data point on the curve is 14, then the scale should extend no longer than 15. Furthermore, the origin or lowest point on the axes does not have to be zero. For example, if the lowest data point on the curve is 4, then the axis can start at 3. Put grid marks on the axes to indicate the scale divisions.

Use complete and consistent axis labels (see Figure 15-3).

- Label each axis with the parameter or variable being measured and the units of measure in parentheses.
• Use initial capital letters only, not all capitals: Time (min), Reaction Temperature (°C), Thickness (µm).
• Place all labels outside and parallel to the axes. Numbers and letters on the abscissa and ordinate should read from left to right and from bottom to top, respectively.
• Do not place arrowheads on the ends of the axis lines.
• Label the tick marks on an axis in type that is one or two points smaller than the axis labels (but not smaller than 7 points in general, 5 points for ACS journals).

➤ Do not draw a box around line-art figures.

➤ For insets, labels, or legends within the figure, use initial capital letters and use the same size type as for the axis labels.

➤ Save electronic figure files with a minimum of white space around the edges.

➤ If you are printing line-art figures for subsequent scanning, always check that the toner or ink cartridge is fresh, and never use a dot-matrix printer.

➤ If you print a hard copy to submit with the electronic file, print it with one figure per page and be sure that the figure number appears on the page.

Working with Photographs and Other Halftone Figures

Good reproduction of photographs begins with good photographs. When you are selecting photographs for figures to accompany your text, consider the following points:

➤ As much as possible, the photograph should show what is important to your text, and only what is important. Clutter and unrelated objects should be cropped out. (This is easy to do with electronic images.)

➤ Photographs always lose some detail in reproduction, so be sure to take the photograph in good focus and, for digital photographs, with sufficient resolution. See Figure 15-4.

➤ Photographs in print will tend to lose contrast and become muddy or gray, so take a few steps to ensure that your photograph has good contrast and tonal definition:
  • Adequately light objects that you are photographing.
  • Place objects on light or dark backgrounds that are plain or solid.
Take several photographs at different settings, so that you can select the one with the best contrast and tonal definition.

Photographs can have tricky copyright and permissions issues. Be sure you understand whether permission is needed to publish the photograph. (See the section called “Common Misconceptions about Copyright” in Chapter 7.)

If you are scanning photographic prints, see Box 15-4.

If you are using a digital camera, select a setting that collects enough digital information. The lowest setting might be sufficient for GIFs, but the higher settings will be necessary for print publication.

Figure 15-4. (A) Example of a photograph with a resolution that is too low for print, so the pixels show as squares, instead of blending to show tones. (B) A similar photograph with a true resolution of 300 ppi.

When you are working with the electronic files of photographs and other halftones, keep the following in mind:

➤ Do not adjust the ppi upward without adjusting the overall dimensions downward. Simply changing the ppi setting from 72 to 300, even if your software allows it, does not put digital information in that was not there before. The file might indicate that the resolution is 300 ppi, but the art will still print as fuzzily as a 72 ppi picture.

➤ You can adjust the ppi downward without changing the overall dimensions. This throws away information that is not necessary and makes a file more portable if, for instance, you scanned at a higher resolution because you were not sure how much you would crop it.

➤ You can switch from RGB to CMYK color modes and vice versa.

➤ If you switch from either RGB or CMYK to B&W, you will probably need to adjust the contrast of your photograph to get the black areas black and the white areas white.

If you are providing photographic prints instead of electronic files, the following points are important to remember:

➤ Submit a good-quality photographic print, preferably not the only original you have. Some publishers try to return original art, but many do not.

➤ Label photographs by writing on an adhesive label (such as a mailing label) first and then applying the label to the back of the photograph, or by writing on a separate sheet of paper and taping it to the back. Writing directly on the back of the photographic print might damage the front: ballpoint pens can break the smooth surface of the photograph, and felt tip pens can bleed through.

➤ Handle photographs with care. Most flaws on a photographic print will be reproduced in the published photograph. You can damage photographs by paper clipping, folding, stapling, or using tape on them. Depending on the amount and location of the damage, you might have to reprint the photograph.

➤ Do not submit prescreened illustrations, that is, illustrations that were scanned from a print source (which is already screened) or scanned using a screen setting.

➤ Do not submit color prints to be reproduced in black and white. Use a professional photo lab to prepare B&W prints from color originals because photo labs use special paper to make B&W prints from color originals.
Working with Grayscale Line Art

Grayscale line art for print publication of such figures as pie charts, bar graphs, and area graphs should be submitted only in an electronic format, preferably EPS. EPS files use mathematical formulas to produce lines and shading, so lines and type are never screened, and gray areas are screened only when the printing plates are made. (Rescreening screened art creates a distortion called moiré.) As a result, the lines in EPS files remain crisp even when the gray tones have been screened.

➤ Always fully embed the fonts or the font outlines in an EPS file. Otherwise, a different font may be substituted at the publisher’s, with unsatisfactory results. Be sure that you have rights to embed the font—you will be safest if you use Times Roman or Helvetica.

➤ Use screen shadings that are different by at least 20 percentage points. For example, you could fill in the sections of a bar graph with 10%, 30%, 50%, 70%, and 100% black. (0%, 20%, 40%, 60%, 80%, and 100% also work well.)

➤ If you choose to screen lines within a line graph (never the axes), assign the lines a 1.5 or 2 point weight, and do not use symbols to mark points on the lines.

Working with Combinations of Type and Photographs

As mentioned in the earlier section, “Types of Figure Artwork”, a photograph that has a simple measuring scale or a few single-letter labels can be adequately handled like other halftones. However, if the photograph (or other halftone artwork) must be accompanied by text to convey meaning, then you should prepare a combo.

One way to do this is to prepare the photograph as a grayscale or color TIFF and then import the photographic image file into a drawing program, such as Illustrator or Freehand. Use the drawing program to add type, lines, axes, tick marks, and so on, and save the file as an EPS with an embedded TIFF.

An alternative is to create the combo in a word-processing program, such as Word or WordPerfect, and then export the page as a PDF file. Simply assembling the type and photograph in the word-processing program and submitting the application (.doc or .wpd) file is seldom acceptable to publishers other than ACS journals.

How To Submit Illustrations

If you follow the recommendations presented in this chapter, you should be well on your way to trouble-free submission of your figure files. Keep the following points in mind for submitting to publishers other than ACS journals.
Publishing with ACS: For manuscripts submitted to ACS journals through Paragon, illustrations should always be embedded in the text document before submission—that is, illustrations should not be submitted as separate files from the text. Illustrations submitted through the Paragon Plus environment can be embedded in the text or supplied separately. Before being embedded, however, the illustrations should be prepared outside the word-processing program to the correct size and resolution as recommended in this chapter. Each illustration should be “inserted” (not “pasted”) into the text document so that it maintains its original resolution, and it should not be adjusted for size after insertion. Graphics taken from Web sites should not be used because, at 72 ppi, their resolution is not adequate for print publication.

For All Figures

➤ Submit a clean photocopy or printout of all figures to accompany your manuscript.

➤ Unless a publisher instructs otherwise, do not put the figures in the midst of text; put them on separate pages at the end.

➤ Put one figure on each page, and label the page with the figure number only. Submit captions as part of your text.

For Electronic Files

➤ Be sure that the art is oriented correctly in the file.

➤ The file name should be brief and consistent, preferably something like Smith_fig02.tiff or Jones_chap5_fig10.eps.

➤ Unless the publisher requests that you submit via a Web site, write the files to a CD, DVD, Zip disk, or 3.5 in. floppy disk. Label the disk with the author name, manuscript title, and general contents, such as manuscript number, figures, tables, and so on.

For Camera-Ready Art

➤ Note the figure number and the first author’s surname either on the back or on the front of each piece of artwork, about 1 in. (2.5 cm) clear of the image area. Do not write on the front or back of the image area; write only in the margins.

➤ Indicate the top of the illustration with the word “top” if the correct orientation is not obvious.
Do not fold or roll artwork or photographs; protect art with cardboard or heavy paper for transport. Do not staple, clip, or punch holes in photographs or any artwork.

How To Prepare Figure Captions

Every figure must have a caption that includes the figure number and a brief, informative description, preferably in nonsentence format.

**GOOD EXAMPLES OF FIGURE CAPTIONS**

Figure 2. Mass spectrum obtained when laboratory ambient air containing 2.5 ppm of $\text{I}$ was introduced into the MS system.

Figure 4. Change in carotenoid contents during maturation of three varieties of grapes: (A) Concord grapes; (B) Thompson seedless; and (C) Chilean red.

Figure 6. Variable-temperature NMR spectra of $\text{3d}$ in $\text{CD}_2\text{Cl}_2$ solution at 500 MHz.

Figure 7. Reaction rate constants as a function of proton affinity for the reactions shown in eqs 5–7: $k_{\text{exp}}$, experimental; $k_{\text{c}}$, calculated.

Figure 1. Specificity of bovine muscle LDH antibodies in a sandwich ELISA. Data represent the averages of three replicates.

If more information is necessary, use complete sentences and standard punctuation. The caption should be understandable without reference to the text (this is essential in Web publishing because the figure may open in a separate frame) and should not include material that is at odds with the text. Use similar wording for captions of related figures.

If a figure contains symbols that require long explanations or has more than four or five symbols, then the key to the symbols will be large and give the artwork a cluttered appearance. In this case, put the key to the symbols in the caption. Make sure that the symbols and abbreviations in the caption agree with those in the figure itself and in the text and that the symbols are typographically available.

Submit the figure captions separately from the artwork, typed double-spaced on a page at the end of the text. Verify that the numbers in the caption agree with the numbers on the figures and in the electronic file names. Bear in mind that figures and captions are handled differently in both Web and print production; captions are usually typeset in a font and size that follow the style of the publication, whereas figures are used as is. If you place the caption on the art, the editors usually will delete it and have the caption typeset according to the publication’s style. At best, this creates additional work and an opportunity for errors to occur; at worst, the presence of captions with the text and on the art may cause confusion if they are inconsistent.
Reproducing Previously Published Materials

To reproduce a figure, photograph, or table that has been published elsewhere, you (the author) must obtain permission in writing from the copyright owner (usually the publisher), and you must submit the written permissions along with your final manuscript. Even if you were the author of the previously published figure or table, you still need written permission from the copyright owner. The only exception is for a work of the U.S. government. See Box 15-7 for examples of credit lines. See also Chapter 7, “Copyright Basics”, for further information.

➤ If you construct a figure or a table from data that were previously published as text or use data from a table to create an original figure, you do not need permission, but you should reference the source of the data (e.g., “Data are from ref 7.”). However, if you are using a portion of a table that has been previously published, even very small portions such as a few data points, permission is needed from the copyright holder.

➤ If you adapt or use only part of a figure or table, permission is still needed. The credit line for adapted material is similar to the credit lines in Box 15-7 except “reprinted” is replaced with “adapted”.

Adapted with permission from ref XX. Copyright Year Copyright Owner’s Name.

Adapted with permission from Author Names (Year of Publication). Copyright Year Copyright Owner’s Name.

➤ If you are thinking about using a previously published figure or table, consider carefully whether citing it as a reference would be adequate.
Box 15-7. Credit Lines in ACS Publications

In ACS publications, credit lines for art reproduced from previously published work appear at the end of the caption in parentheses in one of two formats and follow three possible wordings, depending on the original source:

**Format 1**

*Most publishers:* Reprinted with permission from ref XX. Copyright Year Copyright Owner’s Name.


*Published by ACS:* Reprinted from ref XX. Copyright Year American Chemical Society.

Reprinted from ref 12. Copyright 2005 American Chemical Society.

*Published by the U.S. government:* Reprinted from ref XX.

Reprinted from ref 23.

**Format 2**

*Most publishers:* Reprinted with permission from Author Names (Year of Publication). Copyright Year Copyright Owner’s Name.


*Published by ACS:* Reprinted from Author Names (Year of Publication). Copyright Year American Chemical Society.


*Published by the U.S. government:* Reprinted from Author Names (Year of Publication).


Be sure to check the author guidelines for your publication.
CHAPTER 16

Tables

Betsy Kulamer

This chapter presents guidelines for preparing the tables that accompany a scientific paper for publication. Tables are handled in many ways like figures, so this chapter focuses on the ways in which tables are different and briefly discusses the preparation of tables using word-processing programs.

When To Use Tables

Use tables when the data cannot be presented clearly as narrative, when many precise numbers must be presented, or when meaningful interrelationships can be better conveyed by the tabular format. Tables should supplement, not duplicate, text and figures. (If you are not sure whether you need a table or figure, see Box 15-1.) Examples of material that is best handled as narrative in text are results of IR absorption and NMR chemical shift studies, unless they are major topics of discussion. In many instances, one table with representative data, rather than several tables, is all that is needed to convey an idea.

How To Cite Tables

Like figures, all tables must be called out, that is, mentioned or discussed by name and number in the text.

➤ Capitalize the word “Table” when it is followed by the table number.

➤ Number tables sequentially with arabic or roman numerals, depending on the publication’s style, in order of discussion in the text: Table 2 or Table IV.
Discuss tables sequentially, so that Table 1 is discussed before Table 2, Table 2 before Table 3, and so on.

For good examples of a callout in text, see Chapter 15, Figures, pp 345–346.

How To Prepare Tables

There are two kinds of tables: informal (or in-text) and formal. An informal table consists of three to five lines and is no more than four columns wide; it cannot exceed the width of a text column. Informal tables may be placed in text following an introductory sentence, and each column should have a heading. They are not given titles or numbers, nor do they contain footnotes.

A formal table should consist of at least three interrelated columns and three rows. If you have only two columns, try writing the material as narrative. If you have three columns, but they do not relate to each other, perhaps the material is really a list of items and not a table at all (see the discussion of lists at the end of this chapter). If your table has unusual alignment and positioning requirements, perhaps it should really be a figure. It is important to understand these differences because tables are more expensive to produce than text; the larger the table, the higher the cost. A well-constructed, meaningful table is worth the expense, but anything else is wasteful and does not enhance your paper.

Tables should be simple and concise; arrange all data for optimal use of space. If you have many small tables, consider combining some. Combining is usually possible when the same column is repeated in separate tables or when the same type of material is presented in several small tables. Use consistent wording for all elements of similar or related tables. Be consistent with symbols and abbreviations among tables and between tables and text.

The table width will depend on the widths of its individual columns.

- Generally, tables having up to 6 columns will fit in a single journal column; tables having up to 13 columns will fit in the double-column spread. Tables that exceed the double-column spread will be rotated 90° and set lengthwise on the page.
- In books, tables having up to 8 columns can fit in the page width; tables having 9–12 columns will be set lengthwise on the page. Larger tables can span two pages.
- In all publications, extremely wide tables can cause composition difficulties. In such cases, consider presenting the material as two or more smaller tables.

The style for the individual parts of tables (i.e., the use of capital and lowercase letters and whether the entries are centered or flush left) varies among publications. Consult a recent edition of the journal or the journal’s instructions for authors.
Keep sections of multipart tables at similar widths. Widely divergent section widths within a table waste space and detract from general appearance.

Effective tables are well-designed, so think carefully, first, about the data you need to present and, second, about the best way to present it visually on a page. Sometimes, what looks fine on a letter-size sheet of paper is not practicable for a journal or book page. Sometimes, what you originally conceived as the column headings works better as the row headings. (In general, you should have more row headings than column headings.) Understanding the parts of a table will help you design your tables effectively; they are identified in Figure 16-1.

**Title**

- Give every formal table a brief, informative title that describes its contents in nonsentence format. The title should be complete enough to be understood without referring to the text. Place details in table footnotes, not in the title.

- Begin the table title with the word “Table” and its number, and then continue with the title.

**Column Headings**

Every column must have a heading that describes the material below it. A column heading should not apply to the entire table; information that describes all of the columns belongs in a general table footnote. If a column heading applies to more than one column, use a rule below it that spans the columns to which it applies; this is called a straddle rule. Below the rule, give the specific headings for each column. A unit of measure alone is not an acceptable column heading, unless the column heading appears under a straddle rule.

- Be as succinct as possible, keep column headings to two lines if possible, and use abbreviations and symbols whenever practical.

- Be consistent with the text and with other column headings.

- Define nonstandard abbreviations in table footnotes. Name the variable being measured, and indicate the unit of measure after a comma or slash or within enclosing marks. Use the same style within and among all tables.

**Column Entries**

In many tables, the leftmost column is the stub or reading column. Usually, all other columns refer back to it. Stub entries should be consistent with the text as well as logical and grammatically parallel. Main stub entries may also have sub-entries, which should be indented.
Material in columns can be aligned in various ways; use only one type of alignment per column. Words are usually aligned on the left, and numbers are usually aligned on the decimals, unless they do not have the same units, in which case they are aligned on the left. Use numbers on both sides of a decimal point; numbers less than 1 should have a zero to the left of the decimal point. Columns that are made up of numbers and words together or columns that contain a variety of sizes or types of information might call for alignment on the left, right, or center, depending on the publication’s style.

Do not use ditto marks or the word “ditto” to indicate the same entry in a column; repeat the entry.

Define nonstandard abbreviations in table footnotes.

Try to keep all entries at similar lengths by placing any explanatory material in table footnotes. If you use a dash as a column entry, explain it in a footnote the first time it is used (e.g., “—, too low to be measured.”).

Make sure that all of the columns are really necessary. If there are no entries in most of a column, it probably should be deleted and replaced with a general
table footnote. Alternatively, if the entries in the entire column are the same, the column should be replaced with an appropriate table footnote, such as “In all cases, the value was x.”

**Footnotes**

Table footnotes include explanatory material referring to the whole table and to specific entries. Examples of information that should be placed in general footnotes referring to the whole table are the following: units of measure that apply to all entries in the table, explanations of abbreviations and symbols used frequently throughout the table, details of experimental conditions if not already described in the text or if different from the text, general sources of data, and other literature citations.

Information that should be placed in specific footnotes includes units of measure that are too long to fit in the column headings, explanations of abbreviations and symbols used with only one or two entries, statistical significance of entries, experimental details that apply to specific entries, and different sources of data.

In some publications, such as books, general footnotes and sources are not cited with superscripts; they are labeled “Note” and “Source,” respectively. Specific footnotes are cited with superscripts. In other publications, all footnotes are cited with superscripts. Check the directions for the publication to which you are submitting your paper.

➤ Where superscripts are needed, use superscript lowercase italic letters in alphabetical order, starting from the top of the table and proceeding from left to right.

➤ Write footnotes as narrative and use standard punctuation. Short phrases such as “ND, not determined.” and “x = 23.” are acceptable.

➤ Label each footnote with its superscript letter and group the footnotes together at the end of the table. All footnotes must have a callout in the table title or text.

**Using Word-Processing Software**

When you prepare your tables using word-processing software, a few techniques ensure a smoother transition to either Web or print publication.

➤ In Microsoft Word or WordPerfect, use the software’s table feature, rather than aligning columns using the tab key. Entries arranged with the table feature are more likely to be properly aligned in publication than entries that have been tabbed.

➤ Set up the table in 10 or 12 point type, although 8 point type can be used if necessary. If you need to use type smaller than 8 points to fit your table on a letter-size page, it probably will not fit comfortably on a book or journal page.

➤ Double-space the text in the table.
When you use the table feature, put only one row of entries in each row of
the table. Do not put multiple entries in a single cell by using the hard return.

Avoid using hard returns to add space between rows of the table. If you wish
to show more space than is apparent with double-spacing, use the line format-
ting feature of the word-processing program instead.

How To Submit Tables

If you follow the recommendations presented in this chapter, you should experi-
ence trouble-free submission of your tables. Keep the following points in mind:

Place formal tables after the references at the end of the text file, each on its
own page.

Place informal tables in place within the text.

Submit a printout of tables along with the printout of text if the publisher
requests one.

If a table must contain structures or other art or special symbols, or if a table
has special alignment and positioning requirements, be sure that these are evi-
dent on the printout.

Publishing with ACS: In manuscripts submitted to ACS journals through
Paragon, tables should always be embedded in the text document before
submission, that is, tables should not be submitted as separate files from
the text. Tables in manuscripts submitted through the Paragon Plus envi-
ronment can be embedded in the text or supplied separately.

When To Use Lists

Sometimes you may need to give numerous examples of items, such as chemical
names. In such cases, if there are too many to run into the text, they can be set
as a list in some publications. Put the entries in alphabetical order, unless there
is a reason to do otherwise. A list of names is not truly a figure and not really a
table. Give the list an unnumbered title. In ACS journals, lists may be handled as
informal tables or even as charts.

Potentially Carcinogenic Medicines

azacitidine            cyclophosphamide     methotrexate
azathioprine           cytarabine           nitrofurazone
chloramphenicol        dacarbazine          phenacetin
chlornaphazine         fluorouracil         phenoxybenzamine
The communication of chemical structures is inherently visual, so the language of both chemistry and biochemistry would be sparse without the ability to accurately represent chemistry in a graphical format. Scientific manuscripts today benefit from the visually appealing output of software used to generate structure representations conveying the details of molecular connectivity as well as the details associated with chemical structures, reactions, and schemes. This chapter discusses the use of chemical structures; the related reactions, charts, and schemes, in a scientific manuscript; and methods of preparing and submitting structures for publication. The chapter presents general guidelines; authors should consult with their publishers for specific instructions.

When To Use Structures

A chemical structure is a pictorial representation of the bonding of atoms in a molecule. Chemical structures appear within text at the point at which they are discussed. Structures are numbered sequentially with either arabic or roman numerals; consult the publisher’s guidelines to determine if one is preferred over the other. Generally, there is no need to provide graphical representations of structures for materials that can be accurately represented on one line or in the form of text. For scientific publications, structures should be included for clarity of communication only.

For example, papers describing previously unreported syntheses or reaction sequences, structure–activity relationships, or newly discovered chemical compounds make good use of chemical structure images. Simple chemical struc-
Simple chemical structures can often be represented by a line formula or by the systematic name of the compound, but complex chemical structures depend on structural representations exhibiting the atom–atom connectivity, including the order and stereochemistry of the bonds. Even though a systematic name can accurately describe the chemical structure of paclitaxel, specifically, \((2a\text{R},4\text{S},4\text{a}\text{S},6\text{R},9\text{S},11\text{S},12\text{S},12\text{a}\text{R},12\text{b}\text{S})-6,12\text{b}-\text{diacetoxy}-9-\{[(2\text{R},3\text{S})-3-(\text{benzoylamino})-2-\text{hydroxy}-3-\text{phenylpropanoyl}]\text{oxy}\}-4,11-\text{dihydroxy}-4\text{a},8,13,13-\text{tetramethyl}-5-\text{oxo}-2\text{a},3,4,4\text{a},5,6,9,10,11,12,12\text{a},12\text{b}-\text{dodecahydro}-1\text{H}-7,11-\text{methanocyclodeca}[3,4]\text{benzo}[1,2-\text{b}]\text{oxygen}-12-\text{yl benzoate}\), most chemists would prefer to visualize the structure (shown in Figure 17-1).

**Reminder:** Simple chemical structures can often be represented by a line formula or by the systematic name of the compound, but complex chemical structures depend on structural representations exhibiting the atom–atom connectivity, including the order and stereochemistry of the bonds.

A chemical reaction is a pictorial representation of a change or process. Reactions can be represented with either line formulas or structures; they are placed in text and numbered much like mathematical equations. See pp 272–274 of Chapter 13 for information on how to format chemical reactions.

Groups of structures are called charts. Charts contain representations of multiple structures to facilitate discussion of them. Groups of reactions are called schemes, as shown in Figure 17-2, several reactions can be presented together to show, for example, a step-by-step process. Schemes show action; charts do not.

**How To Cite Structures**

Structures are identified in text with boldface numerals (either Arabic or Roman), boldface alphabet letters (capital or lowercase), or a combination of...
Chemical reactions set as equations should be labeled with lightface roman letters, numerals, or combinations in parentheses in the right margin (see Chapter 13). Depending on the text, it may be appropriate to use one set of labels for both chemical reactions and mathematical equations, or two separate and distinct numbering sequences (for instance, eqs 1, 2, 3, … and reactions I, II, III, …). The numbering sequences for structures and for reactions should always remain separate.

**Reminder:** If a compound is mentioned several times within the text, refer to it only by its label.

Charts are numbered consecutively as Chart 1, Chart 2, and so on, with either arabic or roman numerals. Charts should be labeled with “Chart” and a number; they also may have brief titles and footnotes.
Schemes are numbered consecutively as Scheme 1, Scheme 2, and so on, with either arabic or roman numerals. Schemes should be labeled with “Scheme” and a number; they also may have brief titles and footnotes.

How To Prepare Structures

The quality and size requirements for structures (and, by extension, reactions, schemes, and charts) are similar to those for other illustrations (see Chapter 15). The requirements associated with the representation of structures are supported by most of the software programs for drawing chemical structures (described in Box 17-1). The following guidelines should be used when creating the graphics for chemical structures.

Arrange structures in horizontal rows within the width of a column.

Make the size of the rings and the size of the type proportional. The published size of six-membered rings should be approximately ¼ in. (6.35 mm) in diameter; the published size of five-membered rings should be slightly smaller. The type size should be 5–8 points.

Keep oddly shaped rings and the shapes of bicyclic structures consistent throughout a manuscript. In multiring structures such as steroids, use partial structures that show only the pertinent points.

In three-dimensional drawings, use dashed lines for lines in the background that are crossed by lines in the foreground to give a greater three-dimensional effect. Make lines in the foreground heavier, as shown below.

Center the compound labels (either numbers or letters) just below the structures. If a series of related compounds are being discussed, draw only one parent structure, use a general designation (e.g., R or Ar) at the position(s) where the substituents differ, and specify modifications below the structure.

Reminder: Take care that the structure graphic inserted into your text file is of sufficient resolution, that is, 300 ppi minimum, with 600 or 1200 ppi even better.

For structures mentioned in tables, provide labeled structures as separate artwork (in text or charts), and use only their labels in the table.
Center the reaction arrows vertically on the midline of the structure height and align the centers of all structures. The midline for all structures is the center of the “tallest” structure on the same line.

An example of a correctly drawn reaction is represented below. As shown, the arrow and the one-line structure are centered, top to bottom, in the height of the full structure. The reaction arrow and the plus sign have an equal amount of space on both sides.

Do not waste space, either vertical or horizontal. Use the full column width before starting a new line. A compact presentation is most effective. Avoid using vertical arrows unless it is necessary to portray a cyclic or “square” reaction scheme. Schemes generally read from left to right. As long as the proper sequence is maintained, it does not matter on which line any given structure appears. If a reaction continues to the next line, keep the arrow or other operator on the top line. Refrain from the use of double-column-width charts or schemes unless absolutely necessary because these charts and schemes consume a significant amount of space.

Do not place circles around plus or minus signs.

For most chemical structure drawing programs, it works best to use the copy-and-paste feature to insert the structure drawing into a Microsoft Word document. However, you should take care that the structure graphic inserted into your text file is of sufficient resolution, that is, 300 ppi minimum, with 600 or 1200 ppi even better. The author bears the responsibility to ensure the appropriate insertion.

**Software for Creating Chemical Structures**

A number of chemical structure drawing and rendering programs are available to create structure images of excellent quality and accuracy for inclusion in scientific publications. The most popular commercial structure-drawing packages today include ISIS/Draw, ChemDraw, and ChemSketch (see Box 17-1). Other commercial packages include ChemWindow (now known as DrawIt) and Chemistry 4-D Draw. At this time, Web-based applets do not support the production of graphical output of sufficient quality for most books and journals; other software, such as JMol, should be considered as structure-rendering engines only. Box 17-2 contains parameter settings for ACS publications.
Box 17-1. Software for Drawing Chemical Structures

The following is a selection of commercially available software for drawing chemical structures suitable for publication.


The cost of these software packages can vary considerably based on academic or industrial usage. Fortunately, the cost should not be a barrier to the inclusion of appropriate renderings of chemical structures because several freeware structure-drawing packages are now available for download from the World Wide Web. These include freeware versions of both ISIS/Draw and ChemSketch. A detailed comparison of capabilities for both the freeware and commercial versions of the packages has been made by Tamas Gunda (http://dragon.klte.hu/~gundat/rajzprogramok/dprog.html). This review is an objective comparison, updated on an almost annual basis, of the capabilities of five popular drawing packages [ISIS/Draw, ChemDraw, DrawIt (ChemWindow), ChemSketch, and Chemistry 4-D Draw].

Reminder: The cost should not be a barrier to the inclusion of appropriate renderings of chemical structures because several freeware structure-drawing packages are now available for download.

It is preferable to use one of the drawing packages that offer journal-based templates containing the appropriate bond widths, bond lengths, fonts, and
Box 17-2. Parameter Settings for ACS Publications

At present, ACS journals request that chemical structures be prepared according to the guidelines below. (The guidelines are also available at https://paragon.acs.org/paragon/index.jsp. Click on “Read Author Information,” and then select the appropriate journal for specific information.) The parameters below are specifically for ChemDraw, using the ACS 1996 document settings; authors using other drawing packages should adapt these parameters to their systems. Most commercial and freeware packages allow these settings to be reproduced either by manual settings or by some sort of journal template feature.

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other settings recommended by a particular journal. Using these templates aids in the production of a chemical structure drawing acceptable to the publishers.

How To Submit Chemical Structures

Many common graphical formats can be generated using structure-drawing packages, including TIFF, GIF, and BMP; follow the guidelines for submitting figures presented in Chapter 15. Also, because file formats continue to develop and the preferences of a given publisher can change, authors should check with the publisher’s or journal’s author guidelines for acceptable software and file formats. Box 17-3 shows guidelines for submitting structures to ACS journals.
The visual appeal of a structure or reaction can differ from one software package to another, so authors may wish to interchange data between programs to obtain the best graphical display required for publication. Such an interchange is normally performed using a specific format of the atom–atom connection table known as a molfile. (Information on the MDL molfile format is available at http://www.mdl.com/downloads/public/ctfile/ctfile.pdf.) Such collections may, for example, describe molecules, molecular fragments, substructures, substituent groups, polymers, alloys, formulations and mixtures, and unconnected atoms. Most chemical structure drawing software packages available today allow both import and export of a molfile. An alternative generic file format is CML, the chemical markup language, which takes advantage of the strength of Web-based technologies and is discussed in Chapter 8.

The Future of Representing Chemical Structures

Despite the vast array of tools available today for structure drawing and representation, each tool is lacking in some way for the representation of complete structure space. Small organic molecules have been well supported, but the needs

Box 17-3. Guidelines for Submitting Chemical Structures to ACS Journals

- In manuscripts submitted to ACS journals through Paragon, structures should be embedded in text documents. In manuscripts submitted through the Paragon Plus environment, structures can be embedded in the text or supplied separately.
- Submit graphical images of chemical structures to ACS journals as embedded TIFF files, using a resolution of 300 pixels per inch (ppi) for color and 1200 ppi for black-and-white images.
- ACS journals accept application files (native formats) for several common software programs, including .skc files from ISIS/Draw and .cdx files from ChemDraw.
- Information on submitting chemical structure connection tables is available at https://paragon.acs.org/paragon/application?pageid=content&mid=preferredsoftware.html&parentid=authorchecklist&headername=Preferred%20Software.
- CML is accepted by the ACS Paragon System for submission of supporting information.
of the inorganic, organometallic, and polymer chemist have commonly lagged behind. Chemical structure drawing programs will continue to develop version by version as software vendors deliver an ongoing array of functionality for their customers.

The need to introduce additional flexibility for structure representation will be ongoing, specifically as standards are set for preferred drawing styles by organizations such as IUPAC. A scoping exercise initiated by the IUPAC commission has defined the preferred drawing styles for structure representation to ensure accurate communication of chemical structures. (See http://www.iupac.org/projects/2003/2003-045-3-800.html. The stereo part of this project is now available as provisional recommendations at http://www.iupac.org/reports/provisional/abstract05/brecher_310705.html.) It is likely that publishers will embrace the opportunity to standardize the structure representations within their publications to try to achieve greater homogeneity.

Whereas chemical structures will always be the primary vehicle for visual communication, it is possible that journal articles will be reporting a unique label representing a chemical structure in the near future, especially because this label will already allow the searching of chemical structures contained in publications indexed using Web-based search engines. For more on this, see Appendix 8-1.
CHAPTER 18

Selected Bibliography

References on Scientific Communication

**Technical Writing**


**Style and Usage**


*Webster’s Third New International Dictionary, Unabridged*; Merriam-Webster, Inc.: Springfield, MA, 2002. (Available as a package with a CD and online; see http://www.m-w.com for information on the online product.)


**Style Manuals**


**Mathematics and Numbers**


**Preparing Illustrations**


**References on Chemistry**

### Conventions in Chemistry


### Biochemistry


### Chemical Abstracts

Advice on *Chemical Abstracts* nomenclature is available from the Manager of Nomenclature Services, Department 64, Chemical Abstracts Service, P.O. Box 3012, Columbus, OH 43210. A name-generation service is available through CAS Client Services, Chemical Abstracts Service, P.O. Box 3343, Columbus, OH 43210; e-mail address, answers@cas.org; and URL, http://www.cas.org/Support/client.html.

### Combinatorial Chemistry


### Drug Names

General Chemistry

Chemical Abstracts Index Guide; American Chemical Society: Columbus, OH; Appendix IV (updated periodically).

Inorganic Chemistry


Nomenclature

The International Union of Pure and Applied Chemistry (IUPAC) Nomenclature Documents Home Page on the World Wide Web can be found at http://www.chem.qmw.ac.uk/iupac/. This site contains information on IUPAC itself, the names and publishers of references on chemical nomenclature, and many of the recommendations.

Organic Chemistry

Ring Systems Handbook; American Chemical Society: Columbus, OH, 2003 (and supplements).

Polymer Chemistry

Index

In page references, b indicates boxes, f indicates figures, s indicates schemes, and t indicates tables.

“a”
  before collective nouns, 106
  as gender-neutral alternative, 58
  in titles, 149
  See also Articles (part of speech)
@ in e-mail addresses, 157
“a” and “b” references
  in reference lists, 297–298, 325
  in text citations, 290
“a” vs “an”
  before element symbols, 257
  general usage, 53
  before isotopes, 257, 264
Abbreviations
  “a” vs “an” before, 53
  in abstracts, 22, 158, 160
  academic degrees, 310
  acronyms differentiated from, 158
  for amino acids, 245t–246
  Canadian provinces and territories, 162
  capitalization, 146, 150, 156, 159, 227, 228,
  272
  case sensitivity, 159
  chemical reactions, 272, 273
  commonly used in chemistry, 169–202
  computer and Internet terms, 163–168
  defining, 22, 158, 160, 245, 371, 372, 373
  devising your own, 158, 169
  editorial style overview, 158–162
Abbreviations—continued
  at editor’s discretion, 158, 169
  in equations, 160, 211, 217
  in figures, 225, 365
  in foreign names, 153
  genus name repetition, 160
  in government agency references, 313
  isotopic labeling, 265
  in mathematical copy, 213, 217
  mathematical symbols differentiated from, 160, 211
  for monosaccharides, 243t
  for months, 160–161
  not needing definition, 158–159, 217–218, 260
  for nucleic acids, 244t
  for organic groups, 260
  period use, 118, 119, 223, 294
  plural forms, 161
  for publisher names, 302
  reporting analytical data, 274
  roman type use, 154–155, 159–160, 212–
  213, 216, 271–272
  for saccharides, 243t–244
  in tables, 160, 225, 370, 371, 372, 373
  in titles, 20, 150, 159, 160
  U.S. states and territories, 162
  for volume information in references, 303–304
  See also Acronyms, Chemical Abstracts
  Service Source Index (CASSI)
  abbreviations, Symbols, Units of measure
Absolute configuration
D and L forms, 236, 270–271
R and S forms, 270

Absolute constructions, dangling modifiers compared with, 45, 112

“Abstract”, capitalization in references, 303

Abstracts
abbreviations defined in, 22, 158, 160
abstract number in references, 298–299
datums as alternative, 88–89
mathematical symbols defined in, 211
references to meetings and conferences, 307–308, 321
scientific paper format, 21–22

Abuse, ethical considerations, 74

Academic degrees
“a” vs “an” before, 53
abbreviations, 310
in bylines, 21
thesis levels, 309–310

Acceptance of submissions
communications (journal presentations), 19
manuscripts, 12, 28
notification of, 64
peer-review role, 71

Accepted manuscripts, processing, 33–35
See also Editorial process, Electronic submission of manuscripts

Accession dates, Internet sources, 315, 317–321

Accession numbers, U.S. government publications, 312

Acids, capitalization examples, 237t

Acknowledgments
ethical obligations, 8, 14
scientific paper format, 24

Acrobat Distiller (software), 351
Acrobat Reader (software), 60, 68, 351

Acronyms
abbreviations differentiated from, 158
in abstracts, 22
commonly used in chemistry, 169–202
computer terms, 156, 163–168
editorial style overview, 158–162
period use, 119
for publisher names, 302, 307
See also Abbreviations, Symbols

ACS books
author guidelines, 29, 343
column dimensions, 354t
copyright policy, 30
figure costs, 350
reference format, 24, 287–290
template downloads, 29
See also Copyright, Editorial process, Peer review

ACS committees, capitalization guidelines, 147
ACS Copyright Learning Module Web site, 82
ACS Copyright Office
contact information, 79b, 84b
Copyright Status Form, 86
requesting permission from, 84b
ACS copyright policy, 30, 79b, 82
ACS Copyright Status Form, 86
ACS desk references, 127, 135
ACS governing bodies, capitalization guidelines, 147

ACS journals and magazines
ASAP articles, 34
author guidelines, 29, 343, 381b, 382b
CASSI abbreviations, 288t
column dimensions, 354t
copyright policy, 30
ethical guidelines, 11–16
figure costs, 350
figure guidelines, 343, 347, 351, 364
hazard footnotes in, 23
home pages, 28b
numbers style, 208
parameter settings, 381b
reference format, 24, 287–290, 291
reference management programs, 327
structure guidelines, 381b, 382b
supporting information availability, 25
table guidelines, 374
template downloads, 29
type size, 356
See also Copyright, Editorial process, Peer review

ACS local sections, capitalization guidelines, 147

ACS magazines, See ACS journals and magazines
ACS Paragon Plus System, 30, 364, 374, 382b
ACS Paragon System
electronic submission of manuscripts, 60, 62, 69t
submission of artwork, 30, 364, 374, 382b
ACS periodicals, See ACS journals and magazines
ACS Permission Request Form, 84b
ACS permission request guidelines, 83–86
ACS publications
ASAP articles, 34, 318–319
author guidelines, 29, 343, 381b, 382b
column dimensions, 354t
copyright policy, 30
credit lines in, 367b
figure costs, 350
figure guidelines, 343, 346, 364
numeral and word usage, 206
parameter settings, 381b
ACS publications—continued
reference format, 24, 287–290, 291, 300, 317
template downloads, 29
trademark symbols not used in, 23
type size, 356
See also ACS journals and magazines, Copy-
right, Editorial process, Peer review
ACS Publications Division
ASAP articles, 318
copyright owner rights, 78
Copyright Status Form, 86
requesting permission from, 79b, 83, 84b
Web site, 86
ACS quotation marks policy, 121–122
ACS spelling preferences, 129–133
Active voice, writing style, 42, 54
Adaptation of artwork, 84b, 366
Addition compounds, centered dot use, 261
Addresses, computer, See Electronic mail
(e-mail) addresses, Uniform resource
locator, World Wide Web sites
Adjectives
comma use, 115–116
mathematical operators used as, 219
mathematical symbols used as, 215
phrasal, 149
predicate, 143
proper, 137, 143, 152
trademarks as, 146, 157
as unit modifier element, 139–140, 143
See also Unit modifiers
Adobe software
electronic submission of manuscripts, 61, 68
figure preparation, 350–352, 355b, 363
Advanced Chemistry Development software,
379–380, 380b
“Advances” as CASSI keyword, 306
Adverbs
hyphenation guidelines, 141
semicolon use, 119–120
as unit modifier element, 140
“Affect” vs “effect” or “impact”, 52
Affiliation
company name styling, 162
scientific paper format, 21
Affirmative sentences vs double negatives, 45
Agents, submitting, 62
Agreement, subject–verb, 43–44, 105–108
Alcohols
capitalization examples, 237t
forms for, 234b
Alicyclic compounds, nomenclature, 236
Alignment
chemical structures, 379
columnar material in tables, 370, 372, 373,
374
Alignment—continued
columns containing numbers, 207, 372
superscripts and subscripts (stacking), 269
“All”, subject–verb agreement, 108
“Alpha (α) particle”, capitalization of “p”, 149
“Alpha” vs α, 155
Alphabet, Greek, 214
See also Greek letters
Alphabetizing
CASSI abbreviations, 294
reference citations, 289
reference lists, 325
unnumbered lists, 374
alt infix in copolymer names, 243
“Although” instead of “while”, 46
“a.m.”, 205
American Institute of Physics, 60, 62, 69t
American Library Association, 311
American National Standards Institute
(ANSI), 276
American Society for Testing and Materials,
276
Amino acids
abbreviations, 245–246
small capital letter use, 234, 245, 270
“Among” vs “between”, 51
Ampersand in Web addresses, 156
“an” vs “a”, See “a” vs “an”
Analytical data
reporting, 274–276
as supporting information, 25
See also Data, Physical quantities, SI units,
Units of measure
“And”
vs “and/or”, 56
with author citations in text, 289
as coordinating conjunction, 47, 113, 149
vs en dash, 124–125
number of subject, 106
between numbered items, 209
vs plus sign, 55, 211
slash misused for, 56
vs “with” constructions, 56
“And/or”, 56
“And so forth”, 160
Angle brackets, with crystallographic indices,
268
Angular degree or time symbols, 203, 224
Angular vs linear formulas, 267, 376
Anhydrides, capitalization examples, 237t
Animations, Web-enhanced objects, 25
Anions, charged, 266
Anomeric configuration of saccharides, 243
Anonymity of peer reviewers, 8, 71–72
ANSI, See American National Standards Insti-
tute
Antecedents of pronouns, 45–46, 58

Any”, subject–verb agreement, 108

Apostrophes

plurals

of abbreviations, 161

decades, 205

of mathematical symbols, 211

of numerals used as names, 206

possessives, 127

Apparatus, “Experimental” section contents, 22

“Appendix”, capitalization, 144

Appendixes in scientific papers, 24–25

Application files for artwork

definition, 350

Excel file tips, 353b

PDF file creation, 351

See also Computer file formats, specific applications

Appositives, restrictive and nonrestrictive, 116–117

Aqueous state, indicating in reactions, 272

Ar designation for aromatic substituents, 246, 250

Arabic numerals, See Numerals

Arabic surnames, 152

Area graphs

types of artwork, 347

working with, 363

Arguments (mathematical)

definition, 210

enclosing marks for clarity, 216

spacing considerations, 214, 219

Arialse Systems, editorial systems, 60, 69t

Aromatic compounds, 240

Aromatic substituents, 246, 250

Arrays, mathematical concept, 210

Arrows in reactions, 272–273, 379

Article numbering in references, 297

Article reprints, 35

See also Permissions

Article titles in periodical citations, 291, 292t

Articles (journal), See Journal articles

Articles (part of speech)

“a” vs “an”, 53, 257, 264

at beginning of titles, 20, 154

capitalization in titles and headings, 149

before collective nouns, 106

before element symbols, 257

in foreign names, 152–153

as gender-neutral alternative, 58

before isotopes, 257, 264

“Articles ASAP” page, 34

Artwork

ACS copyright policy, 30

adapted, 84b, 366

Artwork—continued

article reprint costs, 35

editorial process, 29–30, 363–365

embedding requirement, 30, 364, 374

handling tips, 362, 364–365

numbering of, 206, 345, 365

permission requirements, 30, 85b, 366

sizing, 352–354, 355, 370, 373

types of, 29, 347–349

See also Charts, Figures, Illustrations, Photographs, Schemes, Structures, Tables

“As”, capitalization in titles and headings, 149

“As compared to” and “as compared with”, 50

As Soon As Publishable (ASAP) articles, 34, 318–319

“As well as”, 47

Asian surnames, 152–153

Aspartic acid/asparagine mixtures, 245

Assignment of copyright by ACS, See ACS copyright policy

Association of American Publishers, 82

“Assuming” as sentence modifier, 112

“Assure” vs “ensure” or “insure”, 52

Asterisk

for corresponding author information, 21

for excited electronic state, 262

for multiplication in computer languages, 211

ASTM International, citing standards, 276

Astronomical terms, capitalization, 149

“at.”, unit of measure, 118

At symbol (@) in e-mail addresses, 157

Atomic numbers

left subscript use, 262

list of elements, 258t–259t

for unnamed elements, 260

Atomic orbitals, chemical conventions, 256

Atomic substituents or residues, designating, 246, 250

Atomic weights, list of elements, 258t–259t

Atoms

datument validation, 96

electronic configuration, 256–257

isotopic, 265

markup languages and the WWW, 91, 92–94

nuclide descriptors, 261–263

symbols and SI units, 277

Attributes (markup language component), 91–94, 96, 97

Attribution, ethical considerations for, 7

Audience considerations

for draft manuscripts, 28b

in popular science, 16

word choice, 50
Author–date citations
multiple references by same author, 290
reference collation, 290, 325
reference format, 30, 287, 289–290

Author guidelines
ACS publications, 29, 343, 381b, 382b
additions or corrections, 35
CIF format, 286
conventions in chemistry, 255
datument validation, 96
electronic submission of manuscripts, 30, 60, 63
figure submission, 343, 363–365
numeral and word usage, 206
peer-review process, 75
reference format, 31, 291
references to books, 300
standard format, 20, 25, 26, 28–29
structure submission, 381
table preparation, 370

Author home page, 62, 63, 64, 68

Author names in references
books, 300–301
e-mail messages, 322
editorial process overview, 30
organization or committee as author, 301, 307, 308, 312, 321
periodicals, 291, 297–299
reference collation, 290, 325–326
theses, 309
U.S. government publications, 312

Author names in text
byline format, 21, 152
citation guidelines, 30, 287, 289–290
period use and spacing, 119

Author responsibility
checking proofs, 33–35, 36
datument potential, 98–99
datument validation, 96
ethical considerations, 3–8, 13–15, 16, 27
graphics insertion, 379
paperwork submission, 32, 33
peer-review process, 75–76
reference accuracy, 24, 30, 31, 290
See also Author guidelines, Copyright entries, Permissions
Author’s complimentary copy, 35
Author’s proof, 33–35, 36
Authorship
copyright considerations, 79, 81, 86
determining, 6–7, 14, 21
order of names as issue, 6
See also Coauthors, Multiple authors
Auxiliary verbs, in compound sentences, 108

Axes
crystallographic notation, 268, 269
mathematical use and italic type, 212, 223
orbital, 256
scaling and labeling, 225, 359–360

b infix in copolymer names, 243
Bar graphs
color use, 345b
types of artwork, 347
when to use, 344
working with, 363

Base pairs, representation of, 244
“Based on” vs “on the basis of”, 52, 111
Bases, numbering in nucleotide sequences, 244t
“Because” instead of “since”, 46
“Because of” instead of “due to”, 112
Behavioral guidelines, See Ethical guidelines
Beilstein references, 299
Bench>Press (software), 60, 62, 69t
Berkeley Electronic Press, editorial systems, 60
“Beta (β) particle”, capitalization of “p”, 149
“Beta” vs β, 155
“Between” vs “among”, 51
“Between … and”, 125, 209
“bi” in element names, 260
Bias
bias-free language, 57–58
and peer reviews, 9, 15, 75
Bibliographic citations, See Reference entries
Bibliographic indexes, foreign surname format, 152
Bibliographies, abbreviation use in, 160
See also Reference entries
Bibloscape (software), 326–327
Billions, 204
Bin-Hex files, 62
Binomial terms, See Taxonomic terms
Bio-Rad software, 379–380, 380b
Biochemistry, reference format exceptions, 291, 300, 301
Biological structure data sources, 284
Biological test data as supporting information, 25
“Bis” as multiplying prefix, 235
Black-and-white (B&W) mode, 350, 351, 352t, 362
Blackboard boldface letters, 214
blend infix in copolymer names, 243
block infix in copolymer names, 243
BMP format, 381
Boiling points, reporting analytical data, 274
Boldface type
with CASSI abbreviations, 295
chemical name numbering, 206
Boldface type—continued
chemical structure identification, 274, 376–377
combinatorial chemistry representation, 246
for Greek letters, 214
in mathematical copy, 213
references to periodicals, 296
superatom representation, 246
Bonding orbitals, chemical conventions, 256
Bonds
punctuation, 244, 267
symbols, 243, 244
Book as reference
author names, 300–301
book title and editions, 301–302, 306
books with editors, 292t, 300–301, 320
books without editors, 292t, 300, 319–320
chapter title, 301, 306
computer program citation format, 323–324
definition, 323–324
editor names, 300–302, 320
examples, 292t–293t
meetings and conferences, 307–308
miscellaneous information, 305
online books, 293t, 314, 319–320
organization or committee as author, 300, 307
pagination information, 304
place of publication, 303
publisher name, 302–303
series publications, 292t, 304, 305–306
special situations, 305–306
volume information, 303–304, 306
year of publication, 303
See also References
Book titles
in book citations, 301–302, 306
italic type for, 154
in presentation citations, 307–308
U.S. government publications, 312
Books (in general)
artwork sizing, 354, 370, 373
table footnotes, 373
types of, 17–18
word choice, 50
See also ACS books, Manuscript entries, Scientific papers
Borrowed material, See Adaptation of artwork, Copyright, Permissions
"Both", subject–verb agreement, 108
"Both … and", 47
Boughton system, isotopic naming, 265–266
Braces
with crystallographic indices, 268
in mathematical copy, 212, 214, 216
in mathematical equations, 219–220
Braces—continued
nesting order, 216
in set notation, 222
with syllabic portion of chemical names, 240
Brackets, See Angle brackets, Curly brackets, Square brackets
Bragg reflection, crystallography, 267
Branched residues of saccharides, 244
Brand names
editorial style, 157
scientific paper format, 23
in titles, 152
See also Trademarks
Bravais lattices, 269
Breaks at end of line, See Line breaks
Bridged compounds, nomenclature, 236
Browsers, See Web browsers
Bulletin, technical, 292t, 314, 324
Bureau International des Poids et Mesures, 255
"But" as coordinating conjunction, 113
parallel construction, 47, 48
in titles and headings, 149
B&W mode, 350, 351, 352, 362
Bylines
foreign surname format, 152
scientific paper format, 21
See also Authorship
Cadmus Systems, editorial systems, 60, 62, 69t
Callouts, See Citations in text
Cambridge Crystallographic Data Centre, 284, 286
Cambridge Structural Database, 284
Cambridgesoft software, 350–351, 379–380, 381b, 381b, 382b
Camera-ready artwork
definition, 343
preparation guidelines, 346
submission guidelines, 364–365
See also Hard copy
Canada, province and territory abbreviations, 162
Canadian Domestic and Non-Domestic Substance Lists, 254
Canonical building blocks of nucleic acids, 244
Capitalization
abbreviations, 146, 150, 156, 159, 227, 228, 272
amino acid abbreviations, 245
axis labels on figures, 360
case-sensitive abbreviations and symbols, 159
chemical element symbols, 145, 240–241, 257
certain abbreviations, 245
chemical names, 143, 145, 151, 233, 235–241, 237t–239t

Capitalization—continued
chemical reaction types, 273
after colons, 120, 144
company and organizational names, 147
computer and Internet terms, 156, 163–168
computer languages, 155
computer protocols, 156
computer software, 156
event names, 148
“figure”, “table”, “chart”, and “scheme”, 143, 345, 369
parenthetical sentences, 123
parts of a book, 144
planet names, 149
polymer names, 146, 150, 237t, 242–243
professional titles, 147
references to periodicals, 291, 299
regions of the country, 148
SI units, 228
small capital letters, 233, 236, 238t, 245, 270–271
spelling recommendations list, 129–133
surnames, 151–152, 153, 225
taxonomic names, 145–146, 150
in text, 143–149
in titles and headings, 148–151, 227, 237t–239t
trademarks, 147, 157
units of measure, 150, 225, 227
words preceded by element symbols, 145
Captions
abbreviation use, 160
colon use, 120
as copyright ownership indicator, 81
manuscript submission, 364
parallelism, 48
preparing, 355, 365
sizing artwork, 354
symbol keys, 365
Carbohydrates, small capital letter use, 236, 270
Cardinal numbers, 203–204, 308
See also Numbers
CAS, See Chemical Abstracts Service
Cascading Style Sheets (CSS), 90
Case sensitivity for abbreviations, 159
Cases regarding copyright, 80, 82
CASSI, See Chemical Abstracts Service Source Index
Catalysts, indicating in reactions, 272
Cations, charged, 266
“Caution”,”Experimental” section contents, 23
CD-ROM publications
cited as references, 293t, 322–323
illustration preparation, 346
Celsius, capitalization, 225
Centered dot
for bond formation or breaking, 267
in chemical formulas, 260
with compound units of measure, 224
in mathematics, 215, 219
nucleic acid representation, 244
spacing guidelines, 215, 219, 261
Centering of text and artwork, See Alignment
CG Information software, 327
CGS system, background of, 228
“Chapter”, capitalization, 144, 303
Chapter number in book references, 303
Chapter titles
in book references, 301, 306
in U.S. government publications, 312
Charges
electric, 256
ionic, 262, 266
“Chart”, capitalization, 143
Charts
citing, 143
editorial process, 29
groups of structures as, 376, 377, 379
numbering, 206, 377
permissions, 83
titles, 148
types of artwork, 347
when to use, 344
working with, 363
See also Artwork
Check-CIF utility, 63, 286
Checking proofs, 33–35, 36
Chemaxon software, 380, 380b
ChemDraw (software), 350–351, 379–380, 380b, 381b, 382b
Chemical Abstracts (CA)
Boughton system for isotopes, 265
and CAS Registry Numbers, 253, 254
citing references in text, 298–299
datuments as alternative, 89
patent citation format, 310
Chemical Abstracts Service (CAS)
chemical nomenclature, 233
Chemical Registry System, 91, 94, 253–254
Chemical Abstracts Service Source Index (CASSI)
citing references in text, 298–299
meeting and conference presentation citations, 308
publisher names and addresses, 302
sample entry, 340–341
series publications, 306
Chemical Abstracts Service Source Index (CASSI)
abbreviations
of ACS periodicals, 288t
commonly cited journals list, 328–339
government agency references, 313
Chemical Abstracts Service Source Index (CASSI) abbreviations—continued
sample entry, 340–341
series titles, 306
use guidelines, 291, 292–293
Chemical apparatus, describing, 22
Chemical descriptors
capitalization, 145, 238–239, 240
style guidelines, 234–236, 240, 241, 270–271
in titles and headings, 150
types of, 233
See also Stereochemical descriptors
Chemical elements
chemical conventions, 257–261, 264
crystallographic indices, 268
isotopes, 263–266
list, 258–259
nuclide descriptors, 262–263
unnamed, 260
See also Element symbols
Chemical formulas
bonds, 267
Chemical Abstracts index of, 254
chemical conventions, 257–261
concentrations, 271
“Experimental” section contents, 22, 23
isotopic nuclides, 264
linear vs angular forms, 267, 376
nuclide descriptors, 262–263
prefix treatment, 235
roman numerals in, 262
in titles, 20
Chemical inventories, commercial, 254
Chemical kinetics, symbols and SI units,
277–278
Chemical literature, popular, 16
Chemical markup language, See CML
Chemical names
boldface numbering sequence, 206
capitalization, 143, 145, 151, 233, 235–241,
237–239
CAS Registry Numbers, 253–254
components of, 233–240
“Experimental” section contents, 22
hyphenation at end of line, 233, 241,
247–249
hyphenation of prefixes and suffixes, 138,
235–236, 270
isotopic labeling, 264–266
locant and descriptor portion of, 234–240,
238–239
multieword examples, 237
numeral and word usage, 206
punctuation in, 241
specialized groups of chemicals, 242–246
syllabic portion of, 233, 240, 241
Chemical names—continued
as unit modifiers, 141, 143
See also Chemical descriptors, Chemical
nomenclature, Locants
Chemical nomenclature
authoritative sources, 233
and CAS Registry Numbers, 254
published updates, 255
punctuation, 124
roman type use, 212
systematic vs trivial, 22
See also Chemical names
Chemical purity, degree of and criteria for, 22
Chemical reactions
abbreviation use, 272, 273
arrows in, 272–273, 379
concentrations in, 271
displayed vs run in, 272, 376
grouped as schemes, 376, 377
numbering, 272, 377
preparing, 378–381
spacing guidelines, 272, 379
submitting, 381–382
See also Schemes
Chemical Registry System, CAS, 253–254
Chemical research, ethical guidelines, 11–16
Chemical safety information
in abstracts, 21
ethical guidelines, 13
“Experimental” section contents, 23
Chemical structures, See Structures
Chemical symbols
case sensitivity, 159
element names used with, 260
list, 169–202, 258–259
published updates, 255
roman type use, 212, 259
See also Abbreviations, Element symbols,
SI units, Symbols, Units of measure,
specific symbols
Chemical terms
capitalization, 143
datum vocabularies, 97
Greek letter use, 155
hyphenation of prefixes, 137
See also Chemical descriptors, Chemical
names, Chemical nomenclature
Cheminnovation (software), 379–380, 380
Chemistry 4-D Draw (software), 379–380, 380
ChemSet notation, 246, 251–252
ChemSketch (software), 379–380, 380
ChemWindow (software), 379–380, 380
Child elements (markup language compo-
nent), 91, 93
Chime (plug-in), 25
Chinese surnames, 152
Chirality, 270–271
CIF, See Crystallographic information files
Circling of charges, 262
Circuit diagrams as supporting information, 25
“Cis”, italicization and capitalization, 145
Citation manager programs, 326–327
Citations in text
  in abstracts, 22
  of equations, 221
  of figures, 143, 345–346
  of footnotes, 373
  of numbered items, 209
  of structures and schemes, 143, 376–378
  of tables, 143, 369–370
  See also Reference entries
City and state names for place of publication,
  294, 295, 303, 310, 328
Class names (taxonomic), capitalization,
  145–146
Classroom use of copyrighted materials, 80
Clause, definition, 42
CML (chemical markup language)
  datument validation, 96–97
  display of, 94, 96
  examples of, 92–94, 93s
  structure submission, 382
CMYK color mode, 350, 352, 362
“Co.”, 162, 303
co infix in copolymer names, 243
“Co-workers” in textual citations, 289
Coauthors
  ethical obligations, 14
  reference citation wording, 289
  See also Authorship, Multiple authors
Code of Federal Regulations, cited as reference,
  313
CODEN abbreviation, 340
Collating references, 290, 325–326
“Colleagues” in textual citations, 289
Collective nouns, 106–107
Colon
  capitalization after, 120, 144
  with display equations, 221
  in figure captions, 120
  general use, 120
  misuse with components of mixture, 121, 261
  in ratios, 121, 215, 222
  references to U.S. government publications, 312
  between verb or preposition and object, 121
Color artwork, and reprint costs, 35
Color combinations, hyphen use, 125, 140
Color modes, 350–352, 362
Color photographs, 362
Color use in figures, 344, 345b, 346, 350, 353b
Column number in references, 298
Column widths for ACS publications, 354t
Columns in tables, See Tables
Combinatorial chemistry, representation of,
  246, 250–252
Combinatorial libraries, 246, 250–252
Combos (artwork)
  definition, 347
  example, 349f
  file formats, 352r
  working with, 347, 363
Comma
  between adjectives, 115–116
  with appositives, 116–117
  in chemical names, 241
  with compound predicates, 115
  with coordinating conjunctions, 113, 114, 115
  with dates, 118
  and display equations, 221
  with “et al.”, 117–118, 289
  with geographical locations, 118
  with introductory words and phrases, 48, 114
  with “Jr.” and “Sr.”, 117
  between modifier and subject, 110
  with nonrestrictive clauses, 44, 109, 116
  in numbers with five or more digits, 207–208
  in numbers with four digits, 207
  with quotations, 118
  reference citation guidelines, 289–290
  with reference citation numbers, 117, 209, 289
  references to books, 301–302
  references to meetings and conferences, 308–309
  references to periodicals, 296–299
  references to U.S. government publications, 312–313
  serial, 114, 115, 119
  with subordinate clauses, 114
  with subordinating conjunctions, 116
  with two or more adjectives, 115–116
  with units of measure in tables, 371
  verb separated from subject, object, or predicate noun by, 114–115
Commercial chemical inventories of regulatory agencies, 254
Committee on Nomenclature, Terminology, and Symbols of the American Chemical Society, 233
Committees as authors, 301, 307
Communications (journal presentation type), 18–19
  See also Personal communications
Companion publications, cited as reference, 299
“Company”, when to abbreviate and when to spell out, 162
Company logos, copyright basics, 83
Company names
capitalization, 147
MSDS citation, 315
parentheses use, 22, 124
spelling and styling, 127
in titles, 20
when to use, 162
Comparatives, hyphenation in unit modifiers, 141
“Compared to” vs “compared with”, 48, 50
Comparisons
sentence structure, 48–50
word choice, 50–51
Complementary base pairs, representation, 244
Complex sentences, definition, 42
Complimentary copies, 35
Components of mixtures, punctuation, 121, 126, 222, 261
Components of vectors and tensors
italic type use, 212
as mathematical concept, 210
“Composed of” vs “comprised”, 53
Compound predicates, 115
Compound sentences, definition, 42
Compound subjects, 106–107
Compound surnames, hyphenation, 139, 152–153
Compound units of measure, 224, 226, 230r
Compound words
capitalization, 150
definition, 138
hyphenation, 138–139
See also Phrasal verbs, Unit modifiers
Compression of computer files, 62, 351
“Comprised” vs “composed of”, 53
Computer addresses, See Electronic mail
(e-mail) addresses, Uniform resource locator, World Wide Web sites
Computer databases, See Databases
Computer disks for figure files, 364
Computer file formats—continued
reference management programs, 326
structure preparation, 381
word-processing vs PDF files, 60–61
Computer languages
asterisk use, 211
capitalization, 155
Computer monitors
figure preparation issues, 346, 347, 350, 352
font tips, 357b
Computer platforms
PDF file portability, 61
reference manager programs for, 327
templates for, 29
Computer programs, See Software programs
Computer protocols, capitalization, 156
Computer software, See Software programs
Computer terminology list, 163–168
Computerized title searches, 20
Concentrations
conventions in chemistry, 271–272
square brackets use, 124, 271
“Conclusions” section in scientific papers, 7, 23
Conduct guidelines, See Ethical guidelines
Conference proceedings
description, 17
reference format, 292r, 307–309, 321, 323
standard reporting format, 19
Confidentiality of submitted manuscripts, 9, 12, 15, 16, 73–74
Configurational prefixes, chemical names, 235, 241, 243, 245, 270–271
Conflicts of interest
author responsibility to reveal, 8, 12, 15
in editorial process, 12–13
in review process, 9, 15, 75
Confusables words and phrases, 51–53, 111–112
Conjunctions, See Coordinating conjunctions,
Correlative conjunctions, Subordinating conjunctions
Conjunctive adverbs, semicolon use, 119–120
Conseil Européen pour la Recherche Nucléaire (CERN), 89
Constants
defining symbols in text, 211
Greek letter use, 214
italic type use, 212
mathematical abbreviations and symbols, 211, 217–218
as mathematical concept, 210
roman type use, 213
Contents page, hazard footnotes on, 23
Context of research, ethical considerations, 7–9
Continuous-tone art, See Halftone art
Contractions, avoiding, 55
Contracts and copyright, 78, 82
Controlled vocabularies, 97–98
Conventions in chemistry
  atoms and molecules, 261–266
  bonds, 267
  chemical elements and formulas, 257–261
  chemical reactions, 272–274
  chirality, 270–271
  concentration, 271–272
  crystallography, 267–270, 284–286
  electronic configuration, 256–257
  periodic table, 261
  physical quantity symbols, 277–283
  radicals, 266
  reporting analytical data, 274–276
  subatomic particles and quanta, 256
Coordinating conjunctions
  capitalization in titles and headings, 149
  comma use, 113, 114, 115
  definition, 47
  number of subject, 106
  parallelism, 46, 47, 48
Coordination compounds
  capitalization examples, 237t
  square brackets use, 260
Coordination numbers, 270
Copolymer names, 243
Copy editors (in general)
  proofreaders’ marks, 36–39
  role, 33
  See also Editorial process, Editors
Copyright
  basic rights, 79
  copyright notice, 79–80, 83
  duration of, 81, 82
  electronic media, 81, 82, 83
  excerpts, 80
  fair use, 80–81
  font software, 357b, 363
  materials not protected by, 78
  materials protected by, 77–78, 81–82
  misconceptions about, 81–82
  ownership, 78, 81–82, 83, 84b, 86
  permission request guidelines, 83–86, 366
  photographs, 81–82, 361, 366
  public domain status, 81, 83
  registration, 79–80
  reproduced artwork, 29, 83–86, 366
  transferring, 32, 33, 78, 82, 86
  U.S. government works, 81, 366
  U.S. law, 77–82
  works made for hire, 78, 82
  See also Permissions
Copyright infringement, 80, 82, 357b
Copyright laws, 77–82
Copyright notice, 79–80, 83
Copyright policy, ACS publications, 30, 79b, 82
Copyright registration, 80
Copyright Status Form, ACS, 86
Copyright transfer, 32, 33, 78, 82, 86
Corel Draw (software), 351
“Corporation”, when to abbreviate and when
to spell out, 162
Corrections
  to draft manuscripts, 36
  to proofs, 34, 36
  to published manuscripts, 35
  See also Errors entries
Correlative conjunctions
  definition, 47
  parallelism, 46, 47
Correlative constructions, for parallelism, 46, 47
Correspondence (journal presentation type), 18
Corresponding author
  author home page, 62, 63
  contact information, 21
  role in editorial process, 33, 34
Country names for place of publication, 294, 295, 303, 310
Court cases on copyright, 80, 82
Cover letters for manuscripts, 32, 76
Credit lines
  figure captions, 366, 367b
  for previously published material, 84b, 85b, 86, 366, 367b
Critical review of manuscripts, See Peer review
Criticism, in scientific writing, 7–8, 14, 16, 74
Cropping of photographs, 352, 360, 362
cross infix in copolymer names, 243
CrossRef application, 317
Crystallographic information files (CIF)
  basic principles, 284–285
  and datument vocabularies, 97–98
  editors for, 286
  electronic submission of manuscripts, 63
  journal submission requirements, 285–286
  as supporting information, 25
  validation reports, 63, 286
  WWW resources, 284, 286
Crystallography
  CIF format, 25, 63, 97–98, 270, 284–286
  crystallographic point groups, 269
  lattice types, 269
  planes and directions in crystals, 267–268
  space groups, 269–270
  symmetry operations and structural point
groups, 269
  CRYSTMET database, 284
  CSS (cascading style sheets), 90
  Cultivar names, capitalization, 145–146
  Curly brackets, combinatorial chemistry rep-
  resentation, 246, 251–252
Curves, plotting in figures, 358–359
Cyan–magenta–yellow–black (CMYK) color mode, 350, 352, 362
“cyclo” prefix, style for, 236
D in chemical names, 236, 245, 270–271
dA•dT and dG•dC pairings, 244
Dangling modifiers, 45, 109–113
Dashed lines for figures, 345f, 358
for structures, 378
Dashes, See Em dash, En dash
Data (in general)
CIF format requirements, 284–286
CIF terminology, 284–285
embedding in Excel files, 353b
ethical considerations in presentation, 5
reporting analytical data, 274–276
as source of original figure or table, 84b, 366
as supporting information, 25
and types of artwork, 344, 369
See also Databases, Datuments
“Data” as singular or plural noun, 106
Data entry numbers, reference format, 314, 320, 324
Data sets, reference format, 314–315
Databases
CAS Chemical Registry System, 253–254
crystal structure data sources, 284
data set citation, 314
datums as alternative, 89
disclosure of research results via, 16
reference collation and management, 326
reference format, 293t, 318, 320, 324
XML display example, 94, 96
Date of access for Internet reference citations, 315
Dated, comma use, 118
month abbreviations, 160–161
numeral and word usage, 160, 205
See also Year of publication
Datuments
authoring and editing tools, 98–99
cost-saving potential, 99
documents compared with, 87–89, 96
identifier use, 94
markup language display, 94–96
markup language examples, 90–94
markup languages and the WWW, 89–90
as scientific grid component, 99–100
subsets, 94
validation, 96–97
vocabularies, 97–98
“D.C.,” CASSI spacing exception, 294
Deadline concerns, See Timeliness as issue
Decades, numerals and plural forms, 205
Deceased authors, acknowledgment of, 14
Decimals and decimal point use, 208, 372
Declarative sentences period use, 118
writing style, 41–42
Definitions used by markup languages, 93, 97–98
Degree of accuracy, numbers style, 208–209
Degree of rotation, crystallographic point groups, 269
Degree symbol decimals use, 208
not used with kelvin, 227
spacing, 203, 224
Degrees, academic, See Academic degrees
“Delta (Δ),” spelling out, 155
Demonstrations, citation guidelines, 307, 321
Deoxyribonucleic acid, abbreviations, 244t
Dependent clauses, See Subordinate clauses
Derivations, mathematical, 23, 25
Derivative works and copyright, 78
Descriptors, See Chemical descriptors, Nuclide descriptors, Stereochemical descriptors
Designation digits for superatoms, 246, 250–251
Determinants italic type for elements, 212
as mathematical concept, 211
roman type for determinants, 213
Deuterium, representation, 264, 266
Dictionaries
ACS desk references, 127, 135
as CIF component, 97–98, 284
as markup language component, 93, 97
“Different from” in comparisons, 49
Digital Object Identifier (DOI) system, 317, 319
Digital photographs, 360, 361f
See also Photographs
Digits, See Numerals
Dimensions of ACS publications, 354t
Directions in crystals, 267–268
“Discussion” section in scientific papers, 7, 23
Disks for figure files, 364
Display equations
in abstracts, 22
numbering of, 220
punctuation before and after, 221
style and usage guidelines, 211, 218
See also Equations
Displayed chemical reactions, See Chemical reactions
Dissertations, cited as reference, 292t, 309–310, 321, 325
Distiller (software), 351
Ditto marks in tables, 372
Division, slash or negative exponent use, 220, 224
DNA, abbreviations, 244†
Document root elements (markup language component), 91
Document titles, U.S. government publications, 312
DOI (Digital Object Identifier) system, 317, 319
Dollar sign, spacing, 203
Dot, centered, See Centered dot
Dot, superscript, 266
Dot-matrix printers
  avoiding for artwork, 353b, 360
  TrueType font format, 357b
Dot size and spacing in halftone art, 347
Dots per inch (dpi), in figure preparation, 346
Dotted lines in figures, 358
Double-blind peer reviews, 71
Double bonds in chemical formulas, 267
Double negatives, avoiding, 45
Double surnames, hyphenation, 139, 152–153
Doubled letters, hyphenation rules, 136
Draft manuscripts, processing of, 27–31
  See also Editorial process, Electronic submission of manuscripts
Drawing settings for ACS publications, 381b
Drawings, 347
  See also Artwork, Figures, Illustrations, Structures
DrawIt (software), 379–380, 380b
Drug names
  capitalization, 145
  in titles, 20
Dublin Core Schema, 90
“Due to”, 51, 111–112
DVDs, cited as references, 293t, 322–323
e (base of natural logarithm)
  “exp” vs e, 217
  roman type use, 213
“e” for negative electron, 256
“e” or “E” in scientific notation, 210
E prefix in chemical names, 236
“Each”, subject–verb agreement, 107
“Earth”, capitalization, 148
“Ed.” vs “ed.”, 301, 302
EdiKit (software), 60
Editable fonts, description, 357b
Editing services, 75
Edition numbers for books, 301
Editor names in references, 292t, 293t, 300–302, 320
Editorial computer systems, See Electronic submission of manuscripts
Editorial lists, See Lists, editorial
Editorial Manager (software), 60, 62, 69t
Editorial process
  accepted manuscripts, 33–35
  CIF format and text editors, 286
data sheet potential, 98–99
draft manuscripts, 27–31
  editing services, 75
  electronic submissions process, 31, 32, 59–69
  figure submissions, 343, 346–347, 363–365
  final manuscripts, 32–33
  proofreaders’ marks, 36–39
  reference management programs, 326
  review of manuscripts, 31
  structure submissions, 381–382
  table submissions, 374
Editorial style, See specific aspects, e.g., Capitalization
Editors (in general)
  CIF validation reports, 286
  ethical guidelines, 12–13
  proofreaders’ marks, 36–39
  role, 33
  See also Editorial process
Educational use of copyrighted materials, 80
“Effect” vs “affect” or “impact”, 52
“e.g.”, 117, 160
“Either”, subject–verb agreement, 107
“Either … or”, 47
eJournal Press, editorial systems, 60, 69t
EJPress (software), 60, 62, 69t
Electric charges, indicating, 256
Electricity and magnetism, symbols and SI units, 278–279
Electrochemistry, symbols and SI units, 279
Electron charges, indicating, 256
Electron shells and subshells, chemical conventions, 256
Electronic bulletin boards, 16
Electronic file formats, See Computer file formats
Electronic lists and newsgroups, 293t, 322
Electronic mail (e-mail)
  manuscript submission via, 31, 59, 61–64
  messages cited as references, 293t, 316, 322
  permission requests via, 84b
  word usage, 50
Electronic mail (e-mail) addresses
  for author home pages, 62
  for corresponding author, 21
  format of, 157
  line break guidelines, 157
  word choice, 50
Electronic media, See Internet, Web entries, World Wide Web sites
Electronic reprints, 35
Electronic source citation
CD-ROMs and DVDs, 293t, 322–323
computer programs, 314, 323–325
data sets, 314
e-mail messages, 293t, 316, 322
examples, 292t–293t
Internet sources, 292t–293t, 314, 316–322
lists and newsgroups, 293t, 322
online books, 293t, 314, 319–320
online periodicals, 292t, 297, 298, 317–319
Web sites, 293t, 314, 320–321
Electronic submission of manuscripts
acceptance of manuscripts, 64
advantages of, 59
author home page, 62, 63, 64, 68
CIF format issues, 63, 284–286
editorial process overview, 30, 31, 32
format and procedural issues, 61–62
preparation of figures, 343, 346–347, 360, 363–365
preparation of materials, 60–61
preparation of structures, 382b
revision of manuscripts, 63–64
software and URLs for selected systems, 60, 65t–67t
submission process, 63
text and image formats for selected systems, 61, 68, 69t
tracking of manuscripts, 62, 63, 64
Element symbols
capitalization, 145, 240–241, 257
centrations, 271
crystallographic indices, 268
isotope specification, 263–266
in locants and descriptors, 233, 234, 238t, 240
nuclide descriptor specification, 261–263
oxidation number spacing, 262–263
roman type use, 159, 234, 241
spectroscopy data reporting, 276
See also Symbols
Elements, chemical, See Chemical elements
Elements (markup language component), 90–94, 96–97
Elements of determinants and matrices
italic type use, 212
as mathematical concept, 210
Ellipses
in mathematical equations, 219
within quotations, 126
with series items, 127
Elliptical clauses as sentence modifiers, 113
Elsevier software, 379–380, 380b, 381
Em dash
with CASSI abbreviations, 295
for clarity, 126
Em dash—continued
with nonrestrictive clauses, 126
in tables, 372
Embedding
artwork in text, 30, 364, 374
data in Excel files, 353b
font software in files, 357b, 363
En dash
for bonds, 267
between components of mixture, 121, 126, 222, 261
in multiword concepts, 124–125
in phrases used as unit modifiers, 143
with range of three or more items, 117, 125, 209, 289
with reference citation numbers, 117, 209, 289
with surnames, 125, 139
Encapsulated PostScript format, See EPS format
enCIFer program, 286
Enclosing marks
in mathematical copy, 212, 214–216, 217
in mathematical equations, 219–220
nesting order, 216
with ranges in scientific notation, 209
roman type use, 212
in set notation, 222
with syllabic portion of chemical names, 240
with units of measure in tables, 371
See also Angle brackets, Braces, Parentheses, Square brackets
Encyclopedias, citation guidelines, 293t, 305–306, 320
End-of-line breaks, See Line breaks
End-of-line hyphenation, chemical names, 233, 241, 247–249
End-of-line punctuation, display equations, 221
EndNote (software), 326–327
Energy levels, indicating, 256
English units system, background of, 228
“enn” in element names, 260
“Ensure” vs “assure” or “insure”, 52
Enumerated lists, 123, 206–207
Enzymes, 155
Eponyms, capitalization, 144
EPRESS (software), 60
EPS format, 61, 351–352, 357b, 363
“eq” or “eqs”, 221
“Equals” vs equal sign, 211
Equations
abbreviation use, 160, 211, 217
in abstracts, 22
citing in text, 221
centrations in, 271

Equations—continued
definition of variables following, 225
displayed, 22, 211, 218, 220, 221
“Experimental” section contents, 23
identifier use and placement, 220
letters for sequencing, 220
numbering, 206, 220, 272, 377
as part of sentence, 221
running into text, 220
spacing guidelines, 219
See also Structures
Equilibrium reactions, arrows for, 272
Equipment
capitalization of names, 147
identification in text, 22, 23
Errata, publication of, 8, 35
Error analysis, 6
Errors
corrections, 34–35, 36
in manuscript submission, 60
by printers, 34
in references, 24, 30, 31
in research
author obligations, 3–4, 6, 8
editor obligations, 13
peer-review purpose, 72
reader obligations, 9–10
“Erythro”, italicization and capitalization, 145
ESPERE (software), 60
Esters, capitalization examples, 237t
“et al.”, 117–118, 289, 291, 312
Eta (η) in chemical names, 235
“etc.”, 160
Ethers, capitalization examples, 237t
Ethical guidelines
authors, 16
editors, 12–13
purpose of, 11–12
reviewers, 15–16
scientists publishing in popular literature, 16
Ethics in scientific publication
attribute and context concerns, 7–8
author obligations, 3–8, 13–15, 16, 27
authorship determination, 6–7
editor obligations, 12–13
full disclosure of results, 5–6, 8
reader obligations, 9–10
reviewer obligations, 8–9, 15–16, 73, 74, 76
significance and timeliness concerns, 4–5
when to publish, 4–6
European Inventory of Existing Commercial
Chemical Substances, 254
Event names, capitalization, 148
“Ever”, hyphenation in unit modifiers, 141
“Every”, subject–verb agreement, 107–108
Excel (software), 61, 352, 353b
Excerpts, See Extracts (textual)
Excited electronic states, 262
Exclusive rights, copyright ownership, 78
“exp” vs “e”, 217
Experimental details
in scientific papers, 22–23, 25
in tables, 373
Exponents
“exp” vs “e”, 217
negative, for division, 224
scientific notation, 210
after subscripts, 216
Extensible markup language, See XML
Extensible stylesheet language, 90
Extracts (textual)
copyright basics, 80, 83–86
indentation and punctuation, 122
See also Quotations
Extraneous words and phrases
in article titles, 20
examples, 54–55
“f” and “ff” in pagination, 297, 304
Fabrication or falsification of data, 4, 10
Faces, crystallographic notation, 267–269
Fahrenheit, capitalization, 225
Fair use, interpretation, 80–81
Family names (personal), See Surnames
Family names (taxonomic), capitalization, 145–146
Fax, permission requests via, 84b
Federal government publications, See U.S. government publications
Federal Register, cited as reference, 313
Fences, See Enclosing marks
“Few”, subject–verb agreement, 108
“Fewer” vs “less”, 51
Fictitious names, not to be listed as authors, 14
“Figure”, capitalization, 143, 345
Figure captions, See Captions
Figures
abbreviation use, 225, 365
abstract guidelines, 22
ACS copyright policy, 30
adapted, 84b, 366
citing, 143, 345–346
color use, 344, 345b, 346, 350, 353b
combos, 347, 349f, 352f, 363
credit lines, 366, 367b
data set references, 314
definition, 344
directory process, 29–30, 363–365
electronic file formats, 350–352
electronic submission of manuscripts, 61
“Experimental” section contents, 23
greyscale line art, 347, 349f, 352, 363
Figures—continued
halftone art, 347, 348f, 360–362, 363
labeling for editorial processing, 364
line art, 347, 348f, 349f, 352, 354–360, 363
vs lists, 374
numbering, 206, 345, 365
permission requirements, 30, 83–86, 366
photograph reproduction, 360–362, 363
preparing, 343, 346–354, 360
problems to avoid, 358f, 359f, 361f
publication costs, 344
publication medium, 346, 351–352
references in, 370
scanning tips, 353b, 354, 355b, 360, 362
sizing, 352–354, 355
submitting, 343, 346–347, 363–365
as supporting information, 358f, 361f
symbol use, 353b, 356, 358f, 363, 365
type sizes and fonts, 353b, 356b, 357b, 358f,
360, 363, 365
types of artwork, 29, 347–349
Web-enhanced objects, 25–26
when to use, 344, 370
See also Artwork, Captions, Illustrations,
Photographs, Structures
File formats, See Computer file formats
File names for figure files, 364
File transfer protocol sites
cited as reference, 320
electronic submission of manuscripts,
61–64
Filters, reference manager programs, 326–327
Final manuscripts, processing of, 32–33
See also Editorial process, Electronic sub-
mision of manuscripts
Financial aid, “Acknowledgments” section
contents, 24
Firefox Web browser, markup language
display, 94
First person
as gender-neutral alternative, 58
writing style, 43–44
Five-digit numbers, 207–208
5’ to 3’ direction for nucleotide sequences, 244
FIZ Karlsruhe, ICSD database, 284
Flow charts, 347
“fold” as suffix, 138, 205
Fontisworks (software), 60
Fonts
copyrights, 357b, 363
in figures, 356b, 357b, 358f, 363, 365
in structures, 380
for symbols, 365
Footnotes
abbreviation use in, 160
for charts and schemes, 377, 378
Footnotes—continued
for contributor information, 14
for corresponding author information, 21
for hazard indication, 23
for references, 24, 152
in tables, 371, 372–373
“For” as coordinating conjunction, 47, 113
“For example”, 117, 160
Foreign-language journals, cited as reference,
299
Foreign (non-U.S.) patents, 208, 310–311
Foreign phrases as unit modifiers, 139
Foreign surnames, 139, 152–153
Formal names, foreign, 152–153
Formal tables
definition, 370
submitting, 374
See also Tables
Formats
computer files, See Computer file formats
scientific papers, See Standard format for
scientific papers
Formulas, See Chemical formulas
Four-color format, 350
Four-digit numbers, 207
Fractions
vs decimals, 208
hyphenation, 139
numeral and word usage, 205
spacing when built-up, 219
subject–verb agreement, 108
in subscripts and superscripts, 217
Fragmentation of research reports, avoiding,
13–14
Fraud, ethical considerations, 74
Free radicals, 266
Free style format for computer program cita-
tion, 324–325
Freehand (software), 351–352, 363
Freeware drawing programs, 379–381
“From … to”, 125, 209
FTP sites
cited as reference, 320
electronic submission of manuscripts, 61–64
Full disclosure of research results, 5–6, 8
Full papers, See Journal articles
Functions
italic type use, 212
as mathematical concept, 210
spacing considerations, 214–215, 219
G for general labeling, 265
g infix in copolymer names, 243
Galley s, marking of, See Proofreaders’ marks
and sample markups
“Gamma (γ) ray”, capitalization of “r”, 149
“Gamma” vs γ, 155
Gas state, indicating in reactions, 272
Gender-neutral language, 57–58
General chemistry, symbols and SI units, 279–280
Generic names, 23, 157
Generic structures, in combinatorial chemistry, 246, 250–251
Genotypes, italic type use, 154
Genus names abbreviating vs spelling out, 160
capitalization, 145–146, 150
italic type use, 154
Geographical locations
  capitalization, 148
  comma use, 118
  postal abbreviations, 161–162
See also Place of publication
Geometric lines and points, roman type use, 213, 223
Geometric planes, italic type use, 212, 223
GIF format, 351–352, 357b, 361, 381
Giorgi system, background of, 228
Given names
  byline format, 21
  foreign name format, 152
  hyphenation, 139
See also Author names in references, Author names in text, Initials, Personal names
Glutamic acid/glutamine mixtures, 245
“Gold book” (IUPAC), 97
Gossett, W., and Student t test, 223
Government, U.S., See U.S. entries
Graft infix in copolymer names, 243
Grammar overview, 41–50, 105–108
See also specific aspects
Grammatical rank, definition, 46
Grant agencies’ manuscript submission systems, 60, 65, 67t
Grant numbers, in “Acknowledgments” section, 24
Graphic artwork, See Artwork, Illustrations
Graphics Interchange Format, See GIF format
Graphs
  editorial process, 29
  examples, 358f, 359f
  types of artwork, 347
  when to use, 344
  working with, 363
Grayscale line art
  definition, 347
  example, 349f
  file formats, 352
  working with, 347, 363
“Greater than” vs “in excess of” or “over”, 51
Greek letters
  alphabet, 214
  for bonding orbitals, 256
  in Boughton system for isotopes, 266
  for chemical and physical terms, 155
  in locants and descriptors, 233, 235, 238t, 240
  in mathematical copy, 214
  for subatomic particles, 256
  in titles and headings, 150
  in unit modifiers, 142
See also specific letters
Greek multiplying prefixes, hyphenation, 136–137
“Green book” (IUPAC), 255
Grid marks in figures, 359
“Group” as collective noun, 106
  lowercased for periodic table references, 261
Group names, isotope position, 265
Group numbers, periodic table references, 261
Grouping of digits in long numbers, 207–208
Grouping words, 50–51
Gunda, Tamas, software reviews by, 380
H in chemical names, 235
η (eta) in chemical names, 235
Halftone art
  definition, 347
  example, 348f
  working with, 347, 360–362, 363
See also Figures, Photographs
Handbooks
  description, 18
  standard format, 19
Hapticity, η to indicate, 235
Hard copy
  checking proofs, 34b, 36
  figure printing, 353b, 360
  figure submission, 364
  manuscript submission, 31
  proofreaders’ marks and sample, 36–39
  reprint orders, 35
  table submission, 374
Hard returns, avoiding in tables, 374
Hazards, identification of, 13, 21, 23
“He”, gender-neutral alternatives, 57, 58
Headings
  capitalization, 148–151, 227, 237t–239t
  parallelism, 48, 371
Hebrew surnames, 152
Helping verbs, in compound sentences, 108
Helvetica typeface, 356b, 363
Hermann–Mauguin symbols, 269
HighWire Press, editorial systems, 60, 69t

“His”, gender-neutral alternatives, 57, 58
“Home Page” designation for citations, 320
Host organization information for Web sites, 321
HTML (hypertext markup language), 89–90, 98
"http://", See Uniform resource locator
HTTP protocol, electronic submission of manuscripts, 61
Hungarian surnames, 153
Hydrogen, H in chemical names, 235
Hydrogen bonds, representation, 244, 267
Hydrogen ion concentration, negative logarithm of, 271–272
Hydroxide ion concentration, negative logarithm of, 271–272
Hydroxyl group, attachment of, 244
Hyperlinks
reference errors as issue, 24, 30, 31
supporting information availability, 25
Hypertext markup language, 89–90, 98
Hyphenation
ACS desk reference use, 135
in amino acid sequences, 245
in CAS Registry Numbers, 254
with CASSI abbreviations, 295
chemical names at end of line, 233, 241, 247–249
color combinations, 125, 140
compound words, 138–139
e-mail addresses, 157
foreign phrases as unit modifiers, 139
with isotope names or symbols, 264–266
locants and descriptors, 234–236, 240, 241, 270–271
of position numbers, 246
prefixes, 135–137, 152, 240, 247–249
proper nouns and adjectives, 137, 138, 143, 152
spelling recommendations list, 129–133
suffixes, 137–138, 151, 152, 247–249
surnames, 139, 152–153
syllabic portion of chemical names, 233, 240, 241
two-word vs phrasal verbs, 139
unit modifiers, 138, 139–143
with unit of measure, 141–143
Web addresses, 156
“I”, writing style, 43–44
i (imaginary number), 213
“ibid.” in reference lists, 298, 326
“-ics” ending for nouns, 107
ICSD database, 284
“Idem” in reference lists, 298, 326
“Identical to” and “identical with”, 49
Identification numbers, CAS Registry Numbers, 91, 94, 253–254
Identifiers in markup languages, 92, 94
Idioms used in comparisons, 49–50
“i.e.”, 117, 160
“II” or “III” in personal names, 117, 291, 301, 309, 312
“III”, hyphenation in unit modifiers, 141
Illustrations
adapted, 84b, 366
combinatorial chemistry representation, 251
datum potential, 98
editorial process, 33, 363–365
electronic submission of manuscripts, 60, 61, 69t, 364
handling tips, 364–365
labeling for editorial processing, 362, 364
permission requirements, 83–86, 366
prescreened and rescreened, 362, 363
submitting, 363–365
types of, 29, 347–349
See also Artwork, Figures, Photographs
Illustrator (software), 351–352, 363
Image file formats, See Computer file formats
“In” vs “affect” or “effect”, 52
“In”, with titles in reference citations, 300, 301
“In excess of” vs “greater than” or “more than”, 51
“In press” references, 315
“in.”, unit of measure, 118, 223
“Inc.” in publisher name, 303
InChI (International Chemical Identifier), 91, 94, 101–102, 383
“Including”, restrictive and nonrestrictive uses, 116
Indefinite pronouns, subject–verb agreement, 107–108
Independent clauses
definition, 42
semicolon use, 119–120
Independent contractors and copyright, 78
See also Works made for hire and copyright
“Independently”, 55
Index, mathematical concept, 211
Indexes of chemical substances and formulas, 253, 254
Indexing
and abstract content, 21
and byline format, 21
and foreign surname format, 152
and title wording, 20
of U.S. government publications, 312
Web-based search engine use, 383
Indices, crystallographic, 267–268
Infinitive phrases as sentence modifiers, 113
Infinitives
  capitalization, 149
  as sentence modifiers, 113
  split, 43
Informal tables
  definition, 370
  submitting, 374
  See also Tables
Information components, description, 99
Information for authors, See Author guidelines
Information retrieval
  abstract content as factor, 21
  title wording as factor, 20
  See also Databases, Indexing, Literature searches
Initials
  byline format, 21
  in e-mail addresses, 157
  in foreign names, 152, 153
  for genus name, 160
  period use and spacing, 119
  reference format, 153, 291, 301, 309, 312
Ink cartridges for figure artwork, 353b, 360
Inkjet printers
  Excel figure specifications, 353b
  TrueType font format, 357b
Inorganic compounds, capitalization examples, 237f
Inorganic crystal structures, data sources, 284
Inorganic molecules, CIF format requirement, 284
Institutional and organizational names
  byline format, 21
  capitalization, 147
  reference format, 301, 307, 308, 312, 321
  See also Company names, Publisher names
Instructions for authors, See Author guidelines
Instrumental diagrams as supporting information, 25
“Ignore” vs “assure” or “ensure”, 52
Integrity issues, See Ethics entries
Intellectual property and DOI use, 317
  See also Copyright, Patents, Permissions
inter infix in copolymer names, 243
Interchange of structure data, 381
Intermediates, in combinatorial chemistry, 251
Intermetallics, crystal structure data sources, 284
International aspects of research and publishing, 59
International Bureau of Weights and Measures, 255
International Chemical Identifier, See InChI
International CODEN Directory, 340
International Committee on Weights and Measures, 228
International Organization for Standardization (ISO), 255, 276, 294
International System of Units, See SI units
The International System of Units (SI), 255
International Union of Biochemistry and Molecular Biology, 233
International Union of Crystallography (IUCr), 63, 284, 286
International Union of Pure and Applied Chemistry (IUPAC)
  centered dot spacing style, 261
  chemical conventions, 255
  chemical terminology, 97
  compound nomenclature, 233
  and InChI, 101–102, 383
  structure representation standards, 383
  unnamed elements, 260
Internet
  citation of Internet sources, 292t–293t, 314, 316–322
t
  terminology list, 163–168
  See also Electronic source citation, Web entries, World Wide Web sites
Interviews, punctuation, 122
Introductions in scientific papers, 7, 22
Introductory words and phrases, 48, 114
Investigator integrity issues, See Ethics entries
Iodine symbol, avoiding confusion with numerals, 262
Ion concentrations, negative logarithms of, 271–272
Ionic charges, indicating, 262, 266
IR spectroscopy, reporting analytical data, 275
“Is” instead of equal sign, 211
ISIS/Draw (software), 379–380, 380b, 382b
ISO, See International Organization for Standardization
“iso” prefix, style for, 236
Isolation of products and intermediates, 251
Isotopes
  “a” or “an” before, 257, 264
  labeling, 264–266
  mass numbers, 261, 263
  modified vs unmodified compounds, 264
  substituted compounds, 264, 265
Issue information in references, 296
Italic type
  in Boughton system for isotopes, 266
  with CASSI abbreviations, 295
  for chirality symbols and symmetry site terms, 270
  combinatorial chemistry representation, 246
  in copolymer names, 243
  in crystallography, 269–270
  for definitions, 154
  for emphasis, 153
Italic type—continued
for genotypes, 154
for molal, 155
in mathematical copy, 160, 212, 223
for orbital axes, 256
in polycyclic aromatic compounds, 240
for word’s first occurrence, 154

Japanese surnames, 153
Jargon, avoiding, 20, 54
JMol (software), 379, 380b
Joint Photographic Experts Group format, 351, 352, 357b

Japanese surnames, 153
Jargon, avoiding, 20, 54
JMol (software), 379, 380b
Joint Photographic Experts Group format, 351, 352, 357b

Journal articles (in general)
artwork sizing, 354, 370, 373
CIF format, 285–286
description, 18
standard format, 19
structure representation future, 383
translations, 299
word choice, 50
See also ACS journals and magazines, Manuscript entries, Scientific papers

Journal as reference—continued
special situations, 299
volume information, 295, 296, 297–298
See also Periodical as reference, References
Journal editors, See Editors
Journal of Combinatorial Chemistry, 246, 251

Journal as reference—continued
special situations, 299
volume information, 295, 296, 297–298
See also Periodical as reference, References
Journal editors, See Editors
Journal of Combinatorial Chemistry, 246, 251

Journal presentations
standard format, 19–20
types of, 18–19
See also ACS journals and magazines, Manuscript entries, Scientific papers

Journal titles
foreign-language journals, 299
italic type use, 154
series titles as, 306
JPEG format, 351, 352t, 357b
“Jr.” and “Sr.”, 117, 291, 301, 309, 312
Judicial decisions on copyright, 80, 82

Kappa (κ) in chemical names, 235
“Kappa” vs κ, 155
Kelvin, degree symbol not used with, 227
Ketones, capitalization examples, 237–238
Keys to artwork symbols, 356, 357b
Keywords
in article titles, 20
for series publications in CASSI, 306
Kinetics, symbols and SI units, 277–278
Kingdom names (taxonomic), capitalization, 145–146
Kirk-Othmer Encyclopedia, cited as reference, 305–306

Korean surnames, 153

L in chemical names, 236, 245, 270–271
Labeling
of axes on illustrations, 225, 359–360
do of computer disks, 364
of illustrations for editorial processing, 362, 364
isotopic, 264–266
numeral use, 206, 289, 325, 345, 365
of speculations, 7
See also Numbering
Laboratory reagents, See Reagents
Language issues, See Word usage
Laser printers
Excel figure specifications, 353b
TrueType font format, 357b
Latin multiplying prefixes, hyphenation, 136–137

Latin terms
abbreviations, 158–159
plural forms, 128
roman type use, 154
See also Taxonomic terms
Lattices, crystallography, 268, 269
Laue indices, crystallography, 267
Laws
  cited as reference, 313
  copyright laws, 77–82
Laymen, word choice for, 16
Legends for artwork symbols, 356, 365
Length of manuscript, limiting, 5, 25, 32
“Less” vs “fewer”, 51
Letters (journal presentation type), 18
“Levels” with plurals of symbols, 211
Libraries, combinatorial, 246, 250–252
Licensing arrangements and copyright, 82
Ligating atom, κ to designate, 235
Ligation sites, 234
“like”, hyphenation as suffix, 138
Limits, mathematical spacing, 219
Line art
  definition, 347
  example, 348f
  file formats, 352
  working with, 347, 354–360, 363
See also Figures
Line breaks
  e-mail addresses, 157
  equations, 220
  reaction schemes, 379
  Web addresses, 156
Line graphs
  color use, 345b
  examples, 358f
  types of artwork, 347
  when to use, 344
  working with, 363
Line returns, avoiding hard returns in tables, 374
Line styles
  for figures, 345b, 358
  for structures, 378
Line width
  for figures, 353b, 355, 358, 363
  for structures, 378
Linear vs angular formulas, 267, 376
Lines (geometric) in mathematical copy, 213, 223
Liquid state, indicating in reactions, 272
Lists
  numbered, 123, 206–207
  parallelism, 48
  vs tables, 370, 374
See also References, Series items
Lists, editorial—continued
  CASSI journal abbreviations, 328–339
  chemical name hyphenation, 247–249
  computer and Internet terms, 163–168
  geometric notation symbols, 223
  Greek alphabet, 214
  mathematical operators and symbols, 217–218
  multiplying prefixes, 136–137, 240
  non-SI units, 231t, 232t
  physical quantities and symbols, 277–283
  plurals, tricky, 128
  polymer names, 242
  postal abbreviations, 161–162
  prefixes not to be hyphenated, 135–136
  scientific prefixes, 135–136, 235
  set notation symbols, 222
  SI and SI-derived units, 229t–230t
  spelling and capitalization recommendations, 129–133
  statistical symbols, 223
  surnames as modifiers, 152
  surnames as units of measure, 152, 225
  transport properties, 212
  trigonometric and other functions, 213
  unit modifiers, 140
  words and phrases to avoid, 54–55
Literary vs scientific writing, 28
Literature reviews, See Review articles
Literature searches
  author obligation for, 13
  reference management programs, 326
  “Little”, hyphenation in unit modifiers, 141
  Local government publications, cited as references, 313–314
Locants
  capitalization, 145, 238t–239t, 240
  and chirality, 270
  hyphenation, 234–236, 240, 241, 270–271
  and isotopic labeling, 264–266
  for saccharides, 243
  style guidelines, 234–236
  types of, 233
Logarithms of ion concentrations, 271–272
Loose-leaf services, 314
“-ly” words, hyphenation, 141
m for molal, 155
M for molar, 155, 271
Machine-understandable information and data, See Datuments, InChI
Macintosh platform
  reference manager programs for, 327
  templates for, 29
Macromedia software, 351–352, 363
Macromolecular CIF format, 284
Macromolecular structure data sources, 284
Magazines, See ACS journals and magazines, Periodical as reference
Magnetism and electricity, symbols and SI units, 278–279
“Man”, gender-neutral alternatives, 57–58
Manufacturer names, parentheses use, 22, 124
See also Company names
Manuscript Central (software), 60, 62, 69t
Manuscript confidentiality, 9, 12, 15, 16, 73–74
Manuscript format standards, See Standard format for scientific papers
Manuscript marking by proofreaders, 36–39
Manuscript processing stages accepted manuscripts, 33–35
draft manuscripts, 27–31
final manuscripts, 32–33
proofreaders’ marks, 36–39
resubmission of manuscripts, 76
review, 31, 71–76
See also Editorial process, Electronic submission of manuscripts
Manuscript review, See Peer review
Manuscript submission, See Electronic submission of manuscripts, Manuscript processing stages
Manuscript templates, See Templates
"Many", subject–verb agreement, 108
Marking proofs, 34b, 36–39
Markup languages, See Datuments, specific languages
Mass numbers, 261, 263–264
Mass spectrometry, symbols, 266
Mass spectroscopy, reporting analytical data, 275
Material Safety Data Sheets (MSDSs), 292t, 315
Materials, identification in text, 22
"Materials and Methods" sections, 22–23
Mathematical arguments, See Arguments (mathematical)
Mathematical concepts, definitions, 210–211
Mathematical constants
as concept, 210
defining symbols in text, 211
Greek letter use, 214
italic type use, 212
roman type use, 213
standard abbreviations and symbols, 211, 217–218
Mathematical derivations, 23, 25
Mathematical derivatives, 219, 220
Mathematical equations, See Equations
Mathematical expressions in superscripts and subscripts, 217
Mathematical expressions in text numeral and word usage, 205, 206
punctuation, 124
when to use, 220
Mathematical operators
as concept, 210
link breaks after, 220
roman type use, 212
spacing considerations, 214–215, 217, 219, 222
standard abbreviations and symbols,
217–218
See also Mathematical symbols, Minus sign, Plus or minus sign (±), Plus sign, Times sign (×)
Mathematical papers, sentence modifiers in, 112
Mathematical symbols abbreviations differentiated from, 160, 211
case sensitivity, 159
defining in text, 211
italic type use, 160, 212, 216
not needing definition, 211, 217–218
plural forms, 211
spacing as adjectives, 215
specialized notation, 222–223
See also Abbreviations, Mathematical operators, Symbols, Units of measure, specific symbols
Mathematical variables
as concept, 210
definitions after equations, 225
definitions in text, 211
Greek letter use, 214
italic type use, 212
roman type use, 213
spacing between, 215, 219
Mathematics usage and style abbreviations, 211, 217
boldface type, 213
enclosing marks, 214–216, 217
equations, 218–222
geometric notation, 223
Greek letters, 214
italic type, 160, 212, 223
mathematical concept definitions, 210–211
ratio and mixture notation, 222
roman type, 212–213, 214, 223
script and open-faced letters, 214
set notation, 222
spacing, 214–215
statistics, 223
subscripts and superscripts, 216–217
symbols, 211, 217–218
Matrices
boldface type for matrices, 213
italic type for elements, 212
as mathematical concept, 210, 211
roman type for transposes, 213
MDL molfile format, 382
MDL software, 380b
“Me” vs “myself”, 51
Measure, units of, See Units of measure
Mechanics, symbols and SI units, 280
Meeting and conference presentations
reference format, 56–57, 292t, 307–309, 321, 323
standard reporting format, 19
types of books, 17
Meeting references, “Acknowledgments” section contents, 24
Melting points, reporting analytical data, 274
Members, in combinatorial chemistry, 250–252
Merriam-Webster’s Collegiate Dictionary, 127, 135
Metadata
datument as scientific grid component, 99–100
definition, 89–90
Metal-organic crystal structures, data sources, 284
Metals, crystal structure data sources, 284
“Methods” as CASSI keyword, 306
“Methods” sections, 22–23
Metric system, background of, 228
Metric units, technical documents usage, 223
Microsoft font format, 357b
Microsoft software
electronic submission of manuscripts, 61
figure preparation, 352, 353b, 363
structure preparation, 379
table preparation, 373
Miller indices, crystallography, 267
Millions, 204, 210
Minus sign
and chirality, 271
for electric charge, 256
for ionic charge, 262, 266
for optical rotation, 270
as stereochemical descriptor, 236
structure preparation, 379
Minutes symbol, spacing, 203, 224
Mirror plane, crystallographic symbols, 269
Misplaced modifiers, 44
Mixtures
amino acid representation, 244
combinatorial chemistry representation, 246, 250–252
notation, 222
punctuation, 121, 126, 222, 261
MKSA system, background of, 228
mmCIF format, 284
Model numbers
capitalization, 147
numerals used as names, 206
parentheses use, 22
Modeling programs as supporting information, 25
Modification, isotopic, 264
Modifiers
dangling, 45, 109–112
misplaced, 44
prepositional phrase, 49
sentence, 44–45, 112–113
surnames as, 151
See also Adjectives, Unit modifiers
Mol Draw (software), 380b
Molecules
CIF format requirement, 284
datument potential, 88, 99
electronic configuration, 257
InChI identifiers, 91, 94, 101–102
isotopic substitution, 264
markup languages and the WWW, 91, 92–94, 95f, 96
modeling coordinates as supporting information, 25
nuclide descriptors, 261–263
symbols and SI units, 277
molfile format, 382
Monetary values, U.S., 208
Monographs
description, 18
editorial process, 33
standard format, 19
Monosaccharides, abbreviations, 243t
Month abbreviations, 160–161
“Moon”, capitalization, 148
“More than” vs “in excess of” or “over”, 51
“Most”, subject–verb agreement, 108
Movies
still shot permissions, 83
Web-enhanced objects, 25, 26
MSDSs (Material Safety Data Sheets), 292t, 315
“Mu” (µ), spelling out, 155
Multidimensional physical quantities, boldface type use, 213
Multiple authors
author home page, 62
book categories, 17, 18
byline format, 21
editorial process, 33
ethical issues, 6–7, 14
reference citation format, 289
reference collation, 325
references to books, 300–301
Multiple authors—continued
references to periodicals, 291
U.S. government publications, 312
See also Authorship
Multiple prefixes, hyphenation, 136
Multiplication
asterisk use, 211
with compound units of measure, 224
spacing guidelines, 215, 219, 224
Multiplication sign (×), 215
Multiplying prefixes
hyphenation, 136–137, 240
numbers style, 207
SI system, 229\textsubscript{t}
space considerations, 226
Multysyllabic words, hyphenation of suffixes, 138
Multiword concepts, en dash use, 124–125
Mutation, designation of, 246
“My”, writing style, 44
myICAAP (software), 60
“Myself” vs “me”, 51
N- vs N-, when to italicize, 235
\textit{n} before volume number in CASSI, 295
N for normal, roman type use, 155, 271
“Namely”, comma use, 117
Names of persons, See Author names in references, Author names in text, Personal names
Namespaces (CML component), 92
Naming of chemical compounds, See Chemical names, Chemical nomenclature
National Academy of Sciences, 4
National Institute of Standards and Technology, 228, 255
National Institutes of Health, 10
National Science Foundation, 10
Negative electrons, indicating, 256
Negative exponents for division, 224
Negative logarithms of ion concentrations, 271–272
Negative numbers, “to” or “through” with, 125, 209
“Neither”, subject–verb agreement, 107
“Neither … nor”, 47
“neo” prefix, style for, 236
Nesting order for enclosing marks, 216
Net plane, crystallographic symbols, 268–269
Newsgroups, electronic, 293\textsubscript{t}, 322
Newspapers
nonscientific periodicals, 292\textsubscript{t}, 299
special typefaces, 154
“nil” in element names, 260
NMR spectroscopy
reporting analytical data, 274–275
symbols and SI units, 281
“No one”, subject–verb agreement, 107
“No.” in references, 295, 304
“no.” in unit of measure, 118
“Non”, hyphenation as prefix, 137
Non-English terms, plural forms, 128
Non-native English speakers as writers, 28, 75
Non-SI units, lists, 231\textsubscript{t}, 232\textsubscript{t}
“None”, subject–verb agreement, 108
Nonexclusive rights arrangements, 82
Nonhyphenated prefixes, 135–136
Nonrestrictive phrases or clauses
comma use, 44, 109, 116
dash use, 126
grammar overview, 109
Nonscientific periodicals, citing, 292\textsubscript{t}, 299
Nontechnical style for numbers, 203, 204, 205
“Nor” as coordinating conjunction, 47, 113, 149
“Not … but”, 47
“Not only … but also”, 47
Notation
ChemSet notation, 246, 251–252
mathematical, 222–223
scientific, 207, 209–210
See also Abbreviations, Symbols
“Note” line in table footnotes, 373
Notes (journal presentation type), 18
Nouns
“-ics” ending, 107
collective, 106–107
hyphenation and proper nouns, 137, 138
phrasal verbs as, 139
possessives, 127
predicate, 108
proper, 137, 138, 143, 152
as unit modifier element, 139–140, 143
Nuclear chemistry, atomic number use, 262
Nuclear reactions, reaction scheme, 273
Nucleic Acid Database, 284
Nucleic acids, abbreviations, 244
Nucleotides, abbreviations, 244
Nucleosides, abbreviations, 244
Nucleotides, sequence presentation, 244
Nuclide descriptors, atoms and molecules, 261–263
Nuclides, isotopic, 264
Number
of atoms, 263
of the subject, 44, 105–108
“Number” as collective noun, 106
Number–unit of measure combination as singular, 51
Numbered lists, 123, 206–207
Numbering
of charts, 206, 377
of chemical species in text, 206
of equations and reactions, 206, 220, 272, 377
Index ➤ 413

Numbering—continued
of figures, 206, 345, 365
in nucleotide sequences, 244
of references, 206, 289, 325
of schemes, 206, 346, 378
of structures, 206, 246, 346, 375–377
of tables, 206, 369

Numbers
agency report numbers, 312
atomic numbers, 258–259, 260, 262
at beginning of sentence, 204
CAS Registry Numbers, 91, 94, 253–254
charge numbers for ions, 262
chemical concentrations, 271–272
comparison words, 51
coordination numbers, 270
crystallographic point groups, 269
data entry numbers, 314, 320, 324
decimal point guidelines, 208, 372
designation digits for superatoms, 246, 250–251
derivation use, 127
den dash use, 125
for equation labeling, 289
expressions used in mathematical sense, 205
hyphenation of prefixes and suffixes, 51
in locants and descriptors, 233, 234, 236, 238, 240
large numbers, 204, 207–208, 210
mass numbers, 261, 263–264
model numbers, 22, 147, 206
negative, “to” or “through” with, 125, 209
nontechnical style, 203, 204, 205
ordinal numbers, 203–204, 205, 308
oxidation numbers, 262–263
parallelism in sentence, 204
patent numbers, 208, 310
position numbers, 246
position of atoms, 263
quantum numbers, 257
rearrangement, parts of in ranges, 209–210
single, in unit modifiers, 142, 143
of species in reactions, 272
species numbers, 272
spelling out vs numerals, 160, 203–205
of standards, 276
style overview, 207–210
unit of measure spacing with, 203, 223–224, 271–272
See also Fractions, Numerals, Reference citation numbers

Numbers of atoms, subscript use, 263

Numerals—continued
chemical species identification, 206
crystallographic point groups, 269
dates, 160, 205
decimal point guidelines, 208, 372
designation digits for superatoms, 246, 250–251
descriptions use, 127
den dash use, 125
for equation labeling, 289
expressions used in mathematical sense, 205
hyphenation of prefixes and suffixes, 137, 138
in locants and descriptors, 233, 234, 236, 238, 240
mathematical use and italic type, 212
as names, 206
numeral and word usage, 203–207
for oxidation numbers, 262–263
in ranges, 125, 204, 209–210, 296
in ratios, 205
for reference labeling, 206, 289, 325
in series, 123, 127, 204, 206–207, 209
for species numbers, 272
spelling out vs numerals, 160, 203–205
See also Numbers, Reference citation numbers

Numerical roots in element names, 260
“N.Y.”, CASSI spacing exception, 294

O- vs O-, when to capitalize and italicize, 145
O- vs O-, when to italicize, 235
O for products separate, 246, 251, 252
Office of Research Integrity, U.S. Department of Health and Human Services, 4

Official titles
in bylines, 21
capitalization, 147–148

Oligonucleotides, data sources, 284
Oligosaccharides, representation of, 244
“On the basis of” vs “based on”, 52, 111

Online books, 293t, 314, 319–320
See also Web-based publications

“Online” designation for citations, 318–319
Online information, See Electronic source citation, Internet, Web entries, World Wide Web sites
Online periodicals, 292t–293t, 297, 298, 317–319
See also Web-based publications

Online submission of manuscripts, See Electronic submission of manuscripts
“Only”, placement effects on meaning, 45
Ontologies
datum as scientific grid component, 99
definition, 98
Open-faced letters, 214
Open Journal Systems, 60
OpenType fonts, 357b
Operators, See Mathematical operators
Optical rotation in chemical names, 270
"Or"
    vs "and/or", 56
    as coordinating conjunction, 47, 113, 149
    number of subject, 106
    slash misused for, 56
Oral presentations
    citation guidelines, 307, 321
    converted to scientific papers, 57
Orbitals, chemical conventions, 256–257
Order names (taxonomic), capitalization, 146
Ordinal numbers, 203–204, 205, 308
See also Numbers
Organic compounds, capitalization examples, 237t
Organic crystal structures, data sources, 284
Organic groups, common abbreviations for, 260
Organic Syntheses, cited as reference, 305
Organizational names, See Institutional and organizational names
Orientation of artwork on page, 353b, 364, 370
Original research, reports of, See Scientific papers
"Our", writing style, 44
"Over" vs "greater than" or "more than", 51
Overbar for crystallographic point groups, 269
Overview chapters in proceedings volumes, 17
Oxidation numbers, chemical conventions, 262–263
"p" and "pp" in pagination, 304
Page lengths for ACS publications, 354t
Page number citations
    books, 304
    data sets, 314
    DOI use, 317
    numbers style, 208
    periodicals, 296–297
    U.S. government publications, 312
Page proofs, marking of, See Proofreaders’ marks and sample markups
Paper copy, See Hard copy
"Paper" in references, 304
Paper number, references to meetings and conferences, 308
Paper stock for figure artwork, 353b
Paragon Plus System, 30, 364, 374, 382b
Paragon System
    electronic submission of manuscripts, 60, 62, 69t
    submission of artwork, 30, 364, 374, 382b
Paragraphs, numbered, 207
Parallel constructions
    numeral and word usage, 204
    in tables, 48, 371
    writing style, 46–48, 50
Parallel synthesis, description, 252
Parameter settings for ACS publications, 381b
Paraphrasing, ethical considerations, 7
Parent elements (markup language component), 91
Parentheses
    with abbreviations, 158, 160, 225
    in axis labels on figures, 359
    with chemical prefixes, 236
    with chemical reactions, 272, 377
    comma use, 115
    with compound units of measure, 224
    with credit lines, 367b
    with crystallographic indices, 267–268
    with enumerations, 123, 206–207
    with generic names, 23
    for isotopic substitution, 264
    with manufacturer names, 22, 124
    in mathematical copy, 124, 212, 214–216, 219
    in mathematical equations, 219–220
    nesting order, 216
    for oligosaccharides, 244
    with optical rotation indicators, 270
    with oxidation numbers, 262–263
    in polymer or complex chemical names, 146, 151
    with ranges in scientific notation, 209
    reference citation guidelines, 30, 124, 209, 287, 289–290
    references to books, 305
    references to periodicals, 296
    with standard deviations or standard errors, 208–209
    with syllabic portion of chemical names, 240
Parenthetical expressions
    abbreviation use, 160
    capitalization in titles and headings, 151
    comma use, 117
    hyphenation as unit modifiers, 143
    parentheses use, 123
Parenthetical sentences, 123
Part number in book references, 304, 306
Participles as unit modifier element, 140, 142, 143
Particles in foreign names, 152–153
Parts of a book, capitalization, 144
Passive voice
    avoiding, 42, 54
    and dangling modifiers, 109, 110–111
    as gender-neutral alternative, 58
Passwords for author home pages, 62, 68
Past participles as unit modifier element, 142
Past tense, 42–43
Patent numbers
  citation guidelines, 310
  style guidelines, 208
Patents
  cited as reference, 292t, 310–311
  and publication timing, 5
PDF documents
  electronic submission of manuscripts, 60–61, 68
  figure preparation, 351, 353, 357b
  font tips, 357b
Peer review
  author requests regarding, 13, 15–16, 72, 75
  author responsibilities, 75–76
  CIF validation reports, 63, 286
  double-blind reviews, 71
  editorial process, 29, 31, 32
  electronic submission of manuscripts, 31, 59, 60, 63, 68
  encouragement to new investigators, 76
  ethical considerations, 5, 8–9
  ethical guidelines, 15–16, 73, 74, 76
  of journal presentations, 19
  online article regarding, 71
  PDF file suitability, 60–61
  process of, 72–73
  purpose of, 71–72
  review forms, 73
  reviewer ratings, 73
  reviewer responsibilities, 73–74
  topic suggestions, 74b
Peer X-Press (software), 60, 62, 69t
People as photographic subjects, 82, 361
“Per” in spelled-out units of measure, 225, 226
per
  infix in copolymer names, 243
Percent sign, spacing, 203, 224, 271
Period
  with abbreviations or acronyms, 118, 119, 223, 294
  in bridged and spiro alicyclic compounds, 236
  with CASSI abbreviations, 294
  as decimal point, 208
  in declarative sentences, 118
  in e-mail addresses, 157
  with ellipses, 126
  with “et al.”, 289
  with parenthetical sentences, 123
  with quotation marks, ACS policy, 122
  reference citation guidelines, 289–290
  references to books, 301–306
  references to periodicals, 291, 294, 297–299
  references to theses, 309
Period—continued
  references to U.S. government publications, 312–313
  with units of measure, 118, 223
  in Web addresses, 156
“Periodic table”, capitalization, 261
Periodical as reference
  abstracts, 298–299
  article titles, 291, 292t
  author names, 291, 297–299
  CASSI abbreviations, 291, 292–293, 328–339
  CASSI sample entry, 340–341
  examples, 292t–293t
  Federal Register citations, 313
  generic format, 291
  nonscientific magazines and newspapers, 292t, 299
  online periodicals, 292t–293t, 317–319
  organization or committee as author, 307
  pagination information, 296–297
  place of publication, 294, 295
  repeated information, 297
  special situations, 299
  volume information, 295, 296, 297–298
  year of publication, 296, 297–298
See also References
Periodicals, ACS, See ACS journals and magazines
Permission request form, ACS, 84b
Permission request guidelines, ACS, 83–86, 366
Permission request guidelines, non-ACS copyrighted material, 83–86
Permissions
  from ACS Copyright Office, 84b
  ACS copyright ownership benefits, 86
  from ACS Publications Division, 79b, 83, 84b
  credit line preferences, 85b, 86, 367b
  for e-mail and personal communications, 7, 14, 316
  for electronic media, 81, 82, 83
  fair use guidelines, 80–81
  paperwork submission by author, 32, 33
  for photographs of people, 82, 361
  for previously published material, 30, 80, 83–86, 366
  for unpublished material, 7, 12–13, 16
  U.S. government works and public domain, 81
  written request necessity, 83–86, 84b, 366
Person, agreement in, 44
Personal communications
  author obligation to obtain permission, 7, 14
  e-mail citation format, 293t, 316, 322
  general citation format, 292t, 316
See also Electronic mail (e-mail)
Personal criticism, in scientific writing, 7–8, 14, 16, 74

Personal names
byline format, 21
comma use, 117–118
in e-mail addresses, 157
en dash use, 125
foreign name format, 139, 152–153
hyphenation, 139, 152–153
period use, 119
possessives, 127
professional titles with, 21, 147–148, 152
as taxonomic name element, 146
See also Author names in references, Author names in text, Surnames

Personal opinions, avoiding in writing, 44
pH, style for, 155, 271–272
Phenotypes, roman type use, 154
Phosphate group, attachment of, 244
Photocopying copyrighted material
fair use and restrictions, 80
Photographs
color prints, 362
combos, 347, 349f, 352t, 363
copyright, 81–82, 361, 366
domain example, 361f
figure preparation, 360–362, 363
file formats, 350–352, 363
handling and labeling, 362, 364–365
of people, 82, 361
permissions, 82, 83, 361, 366
prescreened, 362
scanning tips, 355b, 362
types of artwork, 347
when to use, 344
See also Artwork, Illustrations
Photon frequency, indicating, 272
Photoshop (software), 350–352, 355b
Phrasal adjectives, 149
Phrasal verbs, 139, 149
Phrases, definition, 42
Phrases to avoid, 54–55
Phylum names, capitalization, 145–146
Physical quantities
boldface type use, 213
italic type use, 216
as mathematical concept, 210
non-SI units, 231t
SI-derived units, 229t, 230t
SI units, 228, 229t
symbols, 277–283
Physical terms, Greek letter use, 155
pi (π)
as mathematical constant, 213
for positive proton, 256
Picas as space measure, 353b, 354t, 356b
Pie charts
color use, 345b
types of artwork, 347
when to use, 344
working with, 363
Piece fractions, when to use, 205
See also Fractions
Pixels per inch as measure, See Resolution of figure files
Place of publication
books, 303
data sets, 314
meetings and conferences, 308
periodicals, 294, 295
theses, 310
U.S. government publications, 312
Plagiarism, ethical considerations, 7, 10, 74
Planck’s constant, indicating, 272
Planes in crystals, 267–269
Planes (geometric) in mathematical copy, 212, 223
Planets, capitalization, 148
Plural forms
of abbreviations, 161
of decades, 205
“eq” or “eqs”, 221
gender-neutral alternative, 58
of mathematical symbols, 211
of numerals used as names, 206
possessives of, 127
taxonomic names, 146, 154
of trademarks, 157
tricky plurals, 128
of units of measure, 224, 225
Plus or minus sign (±)
with standard error or standard deviation, 208–209
as stereoochemical descriptor, 236
Plus sign
vs “and”, 55, 211
with D and L forms, 271
for electric charge, 256
for ionic charge, 262, 266
for optical rotation, 270
as stereoochemical descriptor, 236
structure preparation, 379
“Plus” vs “and”, 55
“p.m.”, 205
pOH, definition, 271
See also pH
Point groups, crystallographic, 269
Points as type size measure
in figures, 353b, 355, 356b, 358, 363
in structures, 378
in tables, 373
Points (geometric) in mathematical copy, 213, 223
“poly” prefix, capitalization, 146, 150
Polyatomic molecules, 257
Polycyclic aromatic compounds, 240
Polymer beads, representation of, 251
Polymer chemistry, symbols and SI units, 281
Polymer names
capitalization, 146, 150, 237, 242–243
copolymers, 243
nucleic acids, 244
roman type use, 242
Pools, in combinatorial libraries, 251–252
Popular literature, ethical guidelines for publication, 16
Portable Document Files, See PDF documents
Position designations for stereochemical descriptors, 270
Position numbers after amino acid abbreviations, 246
Positional prefixes, 145, 235, 238–239, 240
Positions
of atoms, 263
isotopic substitution and labeling, 264, 265
of nuclides, 264
of substituents, 246, 250
on sugar residues, 243
Positive protons, indicating, 256
Possessives, tricky, 127
Postal abbreviations, 161–162, 303, 310
Postdoctoral students and peer review, 9, 75
Poster presentations, citation guidelines, 307, 321
PostScript files, 351–352, 353b
PostScript font format, 357b
Powder diffraction analysis, CIF format requirement, 284
PowerPoint (software), 61, 352, 353b
Powers of 10, 210
ppi as measure, See Resolution of figure files
Predicate adjectives, 143
Predicate nouns, 108
Predicates, compound, 115
Prefixes
to chemical names, 145, 235–236, 240–241, 245, 247–249, 270
to chemical terms, 137
to drug names, 145
hyphenation, 135–137, 152, 240, 247–249
multiplying prefixes, 136–137, 207, 226, 229, 240
to numerals, 137
to proper nouns and adjectives, 137, 152
Prepositional phrases, with split idioms, 49
Prepositions, capitalization in titles and headings, 149, 150
Preprint servers, citing articles retrieved from, 293t, 317, 319
Preprints
citation format, 308
Prescreened illustrations, 362
Present participles as unit modifier element, 142
Present tense, 43
Presentations, See Journal presentations, Meeting and conference presentations, Oral presentations
“Press” in publisher name, 303
Press releases, disclosure of research results, 16
Primed numbering, 244
Primes, spacing considerations, 219
Printed copy, See Hard copy
Printer’s errors, 34
Private communications, See Personal communications
Proceedings volumes
description, 17
reference format, 292t, 307–308, 321, 323
standard reporting format, 19
ProCite (software), 326–327
Production editing, role, 33
See also Editorial process, Editors
Products, in combinatorial chemistry, 246, 251–252
Professional titles
in bylines, 21
capitalization, 147–148
foreign surnames, 152
Programs, computer, See Software programs
“Progress” as CASSI keyword, 306
Pronouns
antecedents of, 45–46, 58
reflexive, 51, 113
Pronunciation, “a” vs “an”, 53, 257, 264
Proofreaders’ marks and sample markups, 36–39
Proofs
checking, 33–35, 36
marking, 34b, 36–39
Proper adjectives, hyphenation, 137, 143, 152
Proper names
adjectives formed from, 144
hyphenation in unit modifiers, 142, 143
hyphenation of prefixes and suffixes, 152
possessives, 127
spelling recommendations, 127
See also Author names in references, Author names in text, Company names, Personal names
Proper nouns, hyphenation, 137, 138, 143, 152
Proportionality in artwork, 355, 356, 358f
See also Sizing of artwork
Protein Data Bank, 284
Proteins, representations of, 154
Proton charges, indicating, 256
Province abbreviations, 161–162
Public domain status, determining, 81, 83
Public pronouncement of research results, 16
Publication information in references, See
Place of publication, Publisher names in references, Year of publication
Publication number, U.S. government publications, 312
Publication phase of editorial process, 34–35
Publication volume information in references, 295, 296, 297–298, 303–304, 306
Publishon (software), 99
“Publish or perish” mentality, 5
PublishASAP (software), 60
Publisher names in references
acronym or abbreviation use, 302, 307
books, 302–303
data sets, 314
meetings and conferences, 308
organization or committee as author, 301, 307, 308, 312, 321
U.S. government publications, 312
Publishers’ guidelines, See Author guidelines
Publishers’ manuscript submission systems, 60, 65–66, 68, 69t
Publishers’ templates, See Templates
Publishing agency information, U.S. government publications, 312
Punctuation
in chemical names, 241
with display equations, 221
e-mail and Web addresses, 156–157
with quotation marks, ACS policy, 121–122
roman type in mathematical copy, 212
unit modifiers with same ending base, 141
See also Colon, Comma, Em dash, En dash, Period, Semicolon, Slash
Pure and Applied Chemistry, 255
Qualifiers of personal names, 117, 291, 301, 309, 312
Quality vs quantity of research, 5
Quanta, chemical conventions, 256
Quantitative analysis, reporting data, 276
Quantities, Units and Symbols in Physical Chemistry, 255
Quantities and Units, 255
Quantum numbers, chemical conventions, 257
Quotation marks
ACS policy on, 121–122
square brackets within, 124
use guidelines, 122
Quotations
added material, 124
colon use, 144
comma use, 118
e llipses use, 126
ethical considerations, 7
interviews, 122
quotation marks use, 121–122, 124
spelling recommendations, 127
See also Extracts (textual)
R and R* prefixes in chemical names, 236, 270
R for sets of substituents or residues, 246, 250–251
“rad” vs “rd” and “radian”, 225
Radiation, symbols and SI units, 282
Radical sign in running text, 217
Radicals, free and charged species, 266
ran infix in copolymer names, 243
Ranges
en dash use, 117, 125, 209, 289
numeral and word usage, 204, 209–210
pagination information in references, 296, 304
units of measure as final item, 226
Rank, grammatical, 46
Rapid Review (software), 60, 62, 69t
RasMol (helper application), 25
Ratios
isotopic, 265
notation, 222
numeral use, 205
punctuation, 121, 222
spacing considerations, 215, 219
“rd” vs “rad” and “radian”, 225
RDF (Resource Description Framework), 99–100
RDF Site Summary (RSS), 100
Reaction names preceded by element symbols, 145, 234, 240–241
Reactions, See Chemical reactions, Nuclear reactions, Schemes
Readers, ethical obligations of, 9–10
Reading column in tables, 371, 372t
Reagents
in combinatorial chemistry, 246, 250–252
identification in text, 22, 23
Recasting sentences
for active voice, 42, 54
to avoid beginning with number, 204
for gender-neutral language, 57–58
words and phrases to avoid, 54
“Recently”, 57
Red–green–blue (RGB) color mode, 350, 352, 362
Refereeing of scientific papers, See Peer review
Reference books used by ACS staff, 127, 135
Reference citation numbers
  formatting, 30, 287
  punctuation, 117, 124, 209, 289
See also Reference numbering
Reference citations in text
  abstract guidelines, 22
  ACS styles, 287–290
  citation manager programs, 326–327
  editorial process, 30–31
  multiple references by same author, 290
  parentheses use, 124
  permission requests, 85b, 366
  placement in sentence, 290
  reporting analytical data, 276
  spacing of page numbers, 208
Reference Manager (software), 326–327
Reference manager programs, 326–327
Reference numbering
  arabic numeral use, 206
  citation guidelines, 289
  collating references, 325
See also Reference citation numbers
References
  “a” and “b” references, 290, 297–298, 325
  abstracts, 298–299, 308, 321
  article titles, 291, 292t
  author names in, See Author names in references
  author responsibility, 24, 30, 31, 290
  books, 290, 292t–293t, 300–306, 319–320, 323–324
  CASSI abbreviations, 291, 292–293, 313, 328–339
  CASSI format for abstracts and proceedings, 308
  CASSI format for computer programs, 324
  CASSI sample entry, 340–341
  chapter titles, 301, 306, 312
  collating, 290, 325–326
  committees as authors, 301, 307
  as copyright ownership indicator, 81
  data sets, 314–315
  editor names, 292t, 293t, 300–302, 320
  editorial process, 30–31
  electronic sources, 292t–293t, 297, 298, 316–325
  errors in, 24, 30, 31
  ethical obligations of authors, 7, 13, 14
  ethical obligations of reviewers, 15
  examples, 292t–293t
  foreign surname format, 152
  government publications, 292t, 295, 311–314, 321
  in illustrations, 289, 373
  management programs for, 326–327
References—continued
  Material Safety Data Sheets, 292t, 315
  material without publication information, 308–309
  meeting and conference proceedings, 56–57, 292t, 307–309, 321, 323
  minimum data, 290, 306, 309, 310
  miscellaneous information, 305
  nontechnical periodicals, 292t, 299
  organizations as authors, 301, 307, 308, 312, 321
  pagination information, 208, 296–297, 304
  patents, 292t, 310–311
  periodicals, 290–299, 292t–293t, 317–319
  place of publication, 295, 303
  placement in manuscript, 24
  publisher names in, See Publisher names in references
  repeated information, 290, 297–298
  series publications, 292t, 304, 305–306
  special situations, 299, 305–306
  technical reports and bulletins, 292t, 314, 324
  theses, 292t, 309–310, 321, 324
  unpublished materials, 308–309, 315–316, 321
  volume information, 295, 296, 297–298, 303–304, 306
  year of publication, 296, 297–298, 303
See also Book as reference, Journal as reference, Periodical as reference
  “References therein”, use in citations, 297
  Reflexive pronouns, 51, 113
  RefWorks (software), 326–327
  Regions of the country, capitalization, 148
  Registered trademark symbol, See Trademark symbol
  Registry Numbers, CAS, 253–254
  Regulatory agencies, commercial chemical inventories of, 254
Rejection of manuscripts
  author guidelines, 75
  ethical considerations, 12
  reasons for, 72, 73, 75–76
“Relative to”, 50
Religious titles in bylines, 21
Repetitive research reports, 5
Report numbers, U.S. government publications, 312
Reports, technical, 292t, 314, 324
Reports of original research, See Scientific papers
Reprinting, permissions for, See Permissions
Reprints, for authors, 35
Reproducibility of results
  ethical considerations, 5–6, 8, 13
  mathematical detail in papers, 23
Reproduction

artwork, 29, 83–86, 366
photographs, 360–362, 363
See also Permissions

Rescreening of illustrations, 363

Research articles, See Journal articles

Research errors, See Errors

Research ethics issues, See Ethics entries

Research grant agencies’ manuscript submission systems, 60, 65, 67

Research reports, See Scientific papers

Residues
in combinatorial chemistry, 246, 250–251
of saccharides, 243, 244

Resolution of figure files

Excel tips, 353b
and file formats, 351–352
graphics from Web sites, 364
photographs and halftone figures, 360–362
and publication medium, 346
scanning tips, 355b
structure graphics, 378, 379, 382b
and type of artwork, 347

Resonance structures, arrows for, 272

Resource Description Framework (RDF), 99–100

“Respectively”, 50, 55

Restriction endonucleases, 155

Restrictive phrases or clauses
comma use, 44, 116–117
grammar overview, 109
writing style, 44

Results integrity issues, See Ethics entries

“Results” section in scientific papers, 7, 23

Review articles
description, 19
standard format, 20, 21

Reviewers of manuscripts
anonymity of, 8, 71–72
author requests regarding, 13, 72, 75
editorial process, 29, 31, 32
electronic submission of manuscripts, 60, 63, 68
ethical considerations, 5, 8–9
ethical guidelines, 15–16, 73, 74, 76
peer-review process, 72–73
responsibilities of, 73–74
selection of, 15, 72–73, 75
See also Peer review

Revising your manuscript, 31, 32b, 63–64, 75–76

RGB color mode, 350, 352, 362
Ribonucleic acid, abbreviations, 244t
Rich Site Summary (RSS), 100
Ring size, structure preparation, 378
RNA, abbreviations, 244t

Roman numerals
vs arabic, 206, 369, 375–378
chemical structure identification, 376–377
for oxidation numbers, 262

Roman type
for chemical compounds, 259
for chemical element symbols, 159, 234, 241
combinatorial chemistry representation, 246
for electronic configuration, 256
in figures, 356b
in locants and descriptors, 234
in mathematical copy, 212–213, 214, 223
for phenotypes, 154
for polymer names, 242
references to books, 301–304, 306
references to meetings and conferences, 308–309
references to periodicals, 291, 297–299
references to theses, 309
references to U.S. government publications, 312
for restriction endonucleases, 155
in subscripts or superscripts, 216
superatom representation, 246
for syllabic portion of chemical names, 233, 240
for trigonometric and other functions, 219, 220
See also Boldface type, Italic type

Rotation
crystallographic point groups, 269
optical, 270
specific, 274

RSS (RDF Site Summary or Rich Site Summary), 100

Rules, straddle, 371, 372t

S- vs S+, when to italicize, 235
S and S* prefixes in chemical names, 236, 270
s orbitals for polymer bead representation, 251

Saccharides, abbreviations, 243t–244

Safety information, See Chemical safety information

Scalar, mathematical concept, 210
Scalar variables, single-letter, 215

Scaling of artwork, See Proportionality in artwork, Sizing of artwork

Scanning programs, 350–352, 355b
Scanning tips for figures, 353b, 354, 355b, 360, 362

Scatter plots, 347

Scheduling concerns, See Timeliness as issue
Schemas
  in CML, 95, 96
  in XML, 90–91, 96, 98, 99
“Scheme”, capitalization, 143
Schemes
  in abstracts, 22
  citing, 143
  CML example, 93
  in combinatorial chemistry, 246, 251–252, 252f
  definition, 376
  editorial process, 29
  footnotes, 378
  numbering, 206, 346, 378
  preparing, 379
  titles, 148, 378
  types of artwork, 347
  when to use, 376, 377f
XML example, 91f
See also Chemical reactions
Schoenflies symbols, crystallography, 269
ScholarOne, editorial systems, 60, 69t
Scientific and technical information exchange (STIX) fonts, 357b
Scientific method, relation to format of scientific paper, 19
Scientific notation, 207, 209–210
Scientific papers (in general)
  book categories, 17–18
  figure use, 343, 344
  journal presentations, 18–19
  standard format, 19–26, 28
  structure use, 375
  table use, 369
  word choice, 50
Scientific publication, ethics in, See Ethical guidelines, Ethics in scientific publication
Scientific publishers, See Publisher entries
Scientific search services, 72
Scientific vs other writing styles, 16, 28, 50
SciFinder (search service), 72, 254
SciFinder Scholar (search service), 72
Screening (printing process), 347, 362, 363
Script letters, 214
Search engines, Web-based, 99, 383
Search services, 72, 254
Seasons, capitalization, 148
Second person as gender-neutral alternative, 58
Seconds symbol, spacing, 203, 224
“Section”, capitalization, 144
Semantic web concept, 89, 96
See also Datums
Semantics, in markup languages, 93–94, 96–99
Semicolon
  between independent clauses, 119–120
  reference citation guidelines, 289
Semicolon—continued
  references to books, 301–305
  references to meetings and conferences, 308–309
  references to patents, 310
  references to periodicals, 291, 297–299
  references to U.S. government publications, 312–313
  with series items, 119
Semiotics, definition, 98
Sentence modifiers, 44–45, 109–113
Sentence structure
  comparisons, 48–50
  parallelism, 46–48, 50
  sentence modifiers, 44–45, 109–113
  split infinitives, 43
  subject–verb agreement, 43–44, 105–108
  verb omissions, 108
  verb tenses, 42–43
  voice, 42
  word order, 45–46
“Separately”, 55
Sequences, nucleotide, 244
Sequential numbering, See Numbering
Serial comma, 114, 115, 119
Serial data sets, 314–315
Serial unit modifiers with same base, 141
“Series” as CASSI keyword, 306
  as collective noun, 306
Series items
  comma use, 114, 115, 119
  ellipses use, 127
  en dash use, 209
  enumerations, 123, 206–207
  numeral and word usage, 123, 127, 204, 206–207, 209
  parallelism, 48
  semicolon use, 119
  units of measure as final item, 226
Series publications, reference format, 292t, 304, 305–306
Series titles, 20, 305–306
Service mark symbol, 157
Set notation, 222
“Several”; subject–verb agreement, 108
Sexist language, avoiding, 57–58
SGML (Standard Generalized Markup Language), 90
Shades of gray, types of artwork, 347
Shading in artwork, 345b, 347, 359f, 363
Shareware, public domain status, 81
SI-derived units, 229t, 230t
SI units
  atomic and molecular, 277
  base units, 228, 229f
SI units—continued
capitalization, 228
chemical kinetics, 277–278
electricity and magnetism, 278–279
electrochemistry, 279
general chemistry, 279–280
mechanics, 280
multiplying prefixes, 229
NMR spectroscopy, 281
polymer chemistry, 281
radiation, 282
space and time, 282
supplementary units, 228, 229
S system background, 228
technical documents usage, 223
thermodynamics, 283
transport properties, 283
Significance of results as publication issue, 4–5
“Similar to” in comparisons, 49
Simple past tense, 43
Simple sentences, definition, 42
Simultaneous manuscript submissions, 5, 14, 16
“Since”, usage guidelines, 46
Single-crystal analysis, CIF format requirement, 284
Single letters or numbers in unit modifiers, 142, 143
Sizing of artwork, 352–354, 355, 370, 373
Sketches, 347
See also Artwork, Figures, Illustrations
Slang, avoiding, 54
Slash
between components of mixture, 121, 126, 222, 261
with compound units of measure, 224, 226
for division, 220, 224
misuse for “and” or “or”, 56
in ratios, 121, 222
spacing considerations, 215, 217, 219–220
and spelled-out units of measure, 225, 226
and units of measure in tables, 371
in Web addresses, 156
Small capital letters in chemical names, 233, 236, 238t, 245, 270–271
Small-molecule crystal structures, data sources, 284
SMILES identifiers, 94
“So” as coordinating conjunction, 47, 113, 149
Software processing of data, See Databases, Dataments
Software programs
capitalization, 156
and CIF format, 285–286
citation management, 326–327
cited as references, 314, 323–325
combinatorial chemistry representation, 251
Software programs—continued
data set citation format, 314
datument potential, 98–99
editorial process, 29, 30
electronic submission of manuscripts, 60, 65t–67t
figure preparation, 343, 346, 350–352, 354, 355b, 363
font copyrights, 357b
structure preparation, 375, 378–383
table preparation, 373–374
Web-enhanced object viewing, 25
See also specific software
Solid state, indicating in reactions, 272
Solid supports, in combinatorial chemistry, 251
Solidus, See Slash
Soluble supports, in combinatorial chemistry, 251
“Some”, subject–verb agreement, 108
Sound files, Web-enhanced objects, 25
Source file formats, See Computer file formats
“Source” line in table footnotes, 373
“sp.”, capitalization, 146
Space and time, symbols and SI units, 282
Space groups, crystallographic, 269–270
Spacing
in CASSI abbreviations, 294
with centered dots, 215, 219, 261
in chemical reactions, 272, 379
in citations of standards, 276
with compound units of measure, 224
between curves in figures, 358
between display fractions, 219
between element and spectral line, 276
with ellipses, 219
with “exp”, 217
around geometric notation, 223
of indices and element names or symbols, 268
mathematical copy guidelines, 210–223
around mathematical functions and operators, 214–215, 217, 219, 222
around mathematical variables, 215
in multiplication, 215, 219, 224
in numbers with five or more digits, 207–208
in numbers with four digits, 207
between numerals and units, 203, 223–224, 271–272
of oxidation numbers, 262–263
with percent sign, 203, 224, 271
of periods after initials, 119
of position numbers, 246
with ratio colons, 215, 219
reference citation guidelines, 117, 209, 289

Spacing—continued
references to books, 304
references to periodicals, 296–297
with slashes, 215, 217, 219–220
in standard deviation or standard error, 208–209
Spanish surnames, 153
Spans, See Ranges
Special characters, See Greek letters, Symbols
Special event names, capitalization, 148
Special materials used in research, distribution of, 8
Special Publication 330, National Institute of Standards, 255
Special sections, standard format, 24–25
Special typefaces, See Boldface type, Italic type
Species names
abbreviating vs spelling out, 160
capitalization, 146, 150
italic type use, 154
Species numbers, 272
Specific rotation, reporting analytical data, 274
Spectra, Web-enhanced objects, 25
Spectral characterization data as supporting information, 25
Spectral information, datument potential, 99
Spectroscopy
data types and representation, 274–276
symbols and SI units, 281
Speculations, labeling in papers, 7
Speeches, converted to scientific papers, 57
Spelling
ACS desk reference use, 127
company names, 127
computer and Internet terms, 163–168
in direct quotations and titles, 127
plurals, 128
possessives, 127
recommended spelling list, 129–133
Spelling out
abbreviations, 158, 160
“equation” in text, 221
fractions, 139
numbers vs numerals, 160, 203–205
taxonomic names, 160
terms in titles, 20
units of measure, 160, 225–226
Spin multiplicity, chemical conventions, 257
Spiro alicyclic compounds, nomenclature, 236
“spiro” prefix, style for, 236
Split idioms, 49
Split infinitives, 43
Sponsors, “Acknowledgments” section contents, 24
“spp.”, capitalization, 146
Square brackets
in bridged and spiro alicyclic compound names, 236
with concentrations, 124, 271
with coordination entities, 260
with crystallographic indices, 268
isotopic labeling, 264–265
in mathematical copy, 124, 212, 214–216
in mathematical equations, 219–220
nesting order, 216
for oligosaccharides, 244
in polycyclic aromatic compounds, 240
in polymer or complex chemical names, 151
with quotation marks, 124
references to online sources, 315, 318
with syllabic portion of chemical names, 240
Square roots, radicals vs superscripts, 217
“Sr.” and “Jr.”, 117, 291, 301, 309, 312
Stacking (aligning) subscripts and superscripts, 269
Staggering (aligning) subscripts and superscripts
conventions in chemistry, 269
for ionic charge, 262
mathematical copy preferences, 216
Standard deviation or standard error, numbers style, 208–209
Standard format for scientific papers
abstract, 21–22
acknowledgments, 24
byline and affiliation, 21
conclusions, 23
discussion, 23
editorial process, 28, 29
experimental details or theoretical basis, 22–23
introduction, 22
references, 24
results, 23
special sections, 24–25
summary, 24
supporting information, 23, 25
title, 20
Web-enhanced objects, 25–26
Standard Generalized Markup Language (SGML), 90
Standards
for chemical symbols and nomenclature, 255
citing in reports, 276
for structure representation, 383
stat infix in copolymer names, 243
State abbreviations
with CASSI abbreviations, 294
U.S. Postal Service, 161–162, 303, 310
State and city names for place of publication, 294, 295, 303, 310
State government publications, cited as references, 313–314
Statistical notation, 223
Stereocchemical descriptors
  in chemical names, 235, 236, 239t, 240
  and chirality, 270
  See also Chemical descriptors, Locants
Stereocchemical prefixes, 235
Stereoisomer descriptors, 145
“Still”, hyphenation in unit modifiers, 141
STIX fonts, 357b
STM publishing, definition, 27, 90
STN International, 254
Straddle rules, 371, 372t
Structural descriptors, 236, 238r–239t
Structural point groups, crystallography, 269
Structural prefixes, chemical names, 235–236
Structure data for crystals, See Crystallographic information files (CIF)
Structure numbers in ChemSet notation, 246, 251–252
Structures
  in abstracts, 22
  CAS Chemical Registry Numbers, 253–254
citing, 376–378
  in combinatorial chemistry, 246, 250–252
description, 375
editorial process, 29
  font selection, 380
  freeware for drawing, 379–381
  future of representation, 382–383
grouped in charts, 376, 379
  as illustrations, 273
InChI identifiers, 101–102, 383
numbering, 206, 246, 346, 375–377
organic group abbreviations, 260
preparing, 378–381
submitting, 381–382
in tables, 374, 378
types of artwork, 347
unique label possibility, 383
Web-enhanced objects, 25
when to use, 375–376, 377f
  See also Artwork, Illustrations
Stub in tables, 371, 372t
Student t test, 223
Subatomic particles, chemical conventions, 256
Subheadings
capitalization, 148
parallelism, 48
Subject–verb agreement, 43–44, 105–108
Submission of manuscripts, See Electronic submission of manuscripts, Manuscript processing stages
Submitted materials in reference lists, 315–316
Submitting agents, 62
Subordinate clauses
  comma use, 114
definition, 42
  as sentence modifiers, 113
Subordinating conjunctions
  comma use, 116
  in comparisons, 48
  in titles and headings, 150
  writing style, 46
Subscripts
  for atomic numbers, 262
  in Boughton system for isotopes, 265–266
  with chemical reactions, 273
  for electronic configuration, 257
  fractions in, 217
  “index” definition, 211
  for ionic charge, 262
  italic vs roman type, 216
  in mathematical copy, 160, 215–217
  mathematical expressions in, 217
  in mathematical symbols, 211
  for number of atoms, 263
  for orbital axes, 256
  plurals of abbreviations ending in, 161
  spacing around operators, 215, 219
  staggering and stacking with superscripts, 216, 262, 269
  in superatom designations, 246, 251
  in titles, 20
Subspecies names
capitalization, 146
italic type use, 154
Substituents, in combinatorial chemistry, 246, 250
Substitution, isotopic, 264–266
Subtitles, capitalization, 148
“Such as”, restrictive and nonrestrictive uses, 116
Suffixes
  hyphenation, 137–138, 150, 152, 247–249
to proper nouns and adjectives, 152
subject–verb agreement, 107
Sugars
  nucleic acid abbreviations, 244t
  saccharide abbreviations, 243t, 244
Summaries, scientific paper format, 24
  See also Abstracts
“Sun”, capitalization, 148
Superatoms, designation, 246, 250–251
Superlatives, hyphenation in unit modifiers, 141
Superscripts
  with chemical reactions, 274
  for corresponding author information, 21
  for electric charge indicators, 256
Superscripts—continued
for electronic configuration, 256–257
fractions in, 217
“index” definition, 211
for ionic charge, 262, 266
italic vs roman type, 216, 373
for mass number, 261, 263
in mathematical copy, 160, 215–217
mathematical expressions in, 217
misuse in isotopic labeling, 265
for oxidation numbers, 262–263
plurals of abbreviations ending in, 161
vs radical signs, 217
reference citation guidelines, 30, 117, 209,
287
references to periodicals, 298
spacing around operators, 215, 219
staggering and stacking with subscripts,
216, 262, 269
in table footnotes, 373
in titles, 20
Supplements, reference format, 296
Supporting information
datument potential, 98–99
datument validation, 96
electronic submission of manuscripts, 63,
69t, 382b
ethical considerations, 5
for lengthy derivations, 23
manuscript revisions, 32b
standard format, 23, 25
Supports, in combinatorial chemistry, 251
Surnames
byline format, 21
capitalization, 151–152, 153, 225
foreign, 139, 152–153
hyphenation, 139, 152–153
as modifiers, 151
reference collation, 290, 325–326
reference format, 153, 291, 301, 309, 312
as units of measure, 151–152, 225
See also Author names in references, Author
names in text, Personal names
Syllabic portion of chemical names, 233, 240,
241
Symbols
atomic and molecular symbols, 277
capitalization guidelines, 145
case sensitivity, 159
chemical kinetics symbols, 277–278
in chemical reactions, 272
commonly used in chemistry, 169–202
crystallography symbols, 269
electricity and magnetism symbols, 278–279
electrochemistry symbols, 279
Symbols—continued
en dash use, 125, 209
in figures, 353b, 356, 358f, 363, 365
font availability, 365
general chemistry symbols, 279–280
for isotopes, 264–266
isotopic labeling, 264–266
mathematical notation, 222–223
mechanics symbols, 280
NMR spectroscopy symbols, 281
for non-SI units, 231t
nonmathematical symbols, 212
for physical quantities, 277–283
polymer chemistry symbols, 281
for positions of atoms, 263
radiation symbols, 282
reporting analytical data, 274
Schoenflies, 269
for SI-derived units, 229t, 230t
for SI units, 229t
sizing of, 353b, 356
space and time symbols, 282
spacing guidelines, 203
in tables, 370, 371, 373, 374
thermodynamics symbols, 283
in titles, 20
for trademarks, 23, 157
transport properties symbols, 283
See also Abbreviations, Acronyms, Chemical
symbols, Element symbols, Mathematical
symbols, specific symbols
Symmetry operations, crystallography, 269
Symmetry site terms and chirality, 270
Symposia, See Meeting and conference pre-
sentations
“Syn”, italicization and capitalization, 145
Synonymous terms, word choice consider-
ations, 50
Syntax and CIF format, 286
Synthesis, combinatorial, See Combinatorial
chemistry
Systematic chemical names, 22
Système International d’Unités, See SI units

  t test, 223
Tab key, avoiding in table preparation, 373
“Table”, capitalization, 143, 369
Table feature of software, 373–374
Tables
abbreviation use, 160, 225, 370, 371, 372,
373
abstract guidelines, 22
adapted, 84f, 366
citing, 143, 369–370
column entry guidelines, 207, 371–374
column heading guidelines, 225, 371, 372t

In The ACS Style Guide; Coghill, A., et al.;
Tables—continued

<table>
<thead>
<tr>
<th>Topic</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>column width guidelines</td>
<td>370</td>
</tr>
<tr>
<td>editorial process</td>
<td>29–30, 33</td>
</tr>
<tr>
<td>“Experimental” section contents</td>
<td>23</td>
</tr>
<tr>
<td>footnotes</td>
<td>371, 372–373</td>
</tr>
<tr>
<td>formal vs informal</td>
<td>370, 374</td>
</tr>
<tr>
<td>vs lists</td>
<td>370, 374</td>
</tr>
<tr>
<td>numbering</td>
<td>206, 369</td>
</tr>
<tr>
<td>parallelism</td>
<td>48, 371</td>
</tr>
<tr>
<td>parts of, 371, 372</td>
<td></td>
</tr>
<tr>
<td>permission requirements</td>
<td>83–86, 366</td>
</tr>
<tr>
<td>preparing</td>
<td>370–374</td>
</tr>
<tr>
<td>references in</td>
<td>289, 373</td>
</tr>
<tr>
<td>repeated entries</td>
<td>372</td>
</tr>
<tr>
<td>row heading guidelines</td>
<td>371</td>
</tr>
<tr>
<td>section heading guidelines</td>
<td>48</td>
</tr>
<tr>
<td>section widths</td>
<td>371</td>
</tr>
<tr>
<td>sizing</td>
<td>370, 373</td>
</tr>
<tr>
<td>standard deviations or standard errors</td>
<td>209</td>
</tr>
<tr>
<td>structures in</td>
<td>374, 378</td>
</tr>
<tr>
<td>submitting</td>
<td>374</td>
</tr>
<tr>
<td>as supporting information</td>
<td>25</td>
</tr>
<tr>
<td>symbol use</td>
<td>370, 371, 373, 374</td>
</tr>
<tr>
<td>titles</td>
<td>148, 371, 372t</td>
</tr>
<tr>
<td>typesetting cost</td>
<td>370</td>
</tr>
<tr>
<td>unit of measure guidelines</td>
<td>207, 225, 371, 373</td>
</tr>
<tr>
<td>when to use</td>
<td>344b, 369, 370</td>
</tr>
<tr>
<td>word-processing software use</td>
<td>373–374</td>
</tr>
</tbody>
</table>

**See also**

Artwork

Tagged Image File Format, See TIFF format

Tags, markup described, 89

HTML limitations, 90

“tag soup” problem, 93

**See also** Datums

“Taking” as sentence modifier, 112

Tangible medium of expression, definition, 77

Tarred files, 62

Taxonomic terms abbreviating vs spelling out, 160

capitalization, 145–146, 150

italic type use, 155, 160

Technical editing datum potential, 98–99

editing services, 75

reference accuracy, 30

role, 33

**See also** Editorial process, Editors

Technical reports and bulletins, reference format, 292t, 314, 324

Television commercials, still shot permissions, 83

Telnet sites, cited as reference, 320

Temperature, units of, See Units of temperature

Temperature scale names, capitalization, 225

**Templates**

editorial process, 29

electronic submission of manuscripts, 60

reference management programs, 326–327

standard format, 20

structure preparation, 380–381

Temple Peer Review Manager (software), 60

Tenses, 42–43

**Tensors**

boldface type for tensors, 213

definition, 210

italic type for components, 212

**Typesetting cost**

**Unit of measure guidelines** 207, 225, 371, 373, 378

**Units of temperature**

“Than” in comparisons, 48

“That” antecedent clarity, 46

with restrictive clauses, 109

“That is”, 117, 160

“The” before collective nouns, 106

as gender-neutral alternative, 58

in journal names, 294

in titles, 20, 149, 154

Theoretical papers, standard format, 20, 23

Thermodynamics, symbols and SI units, 283

Theses, cited as reference, 292t, 309–310, 321, 325

“This”, antecedent clarity, 46

Thomson Scientific products, 327

Three-dimensional art, structure preparation, 378

“Through”, vs en dash, 125, 209

Tick marks in figures, 353b

TIFF format, 61, 351–352, 353b, 357b, 363, 381, 382b

Tilde (~) for polyatomic molecules, 257

Time, units of, See Units of time

Time and space, symbols and SI units, 282

Timeliness as issue

ASAP articles, 34, 318–319

for authors, 4–5, 75

checking proofs, 33, 34

datum potential, 99

for editors, 12

and full disclosure, 5–6

and nonstandard formats, 20

for peer reviewers, 9, 16, 73

permission requests, 30, 84–86

and significance of results, 4–5

and word choice, 57

“Times”, nonmathematical sense, 205
Times New Roman typeface, 357b
Times Roman typeface, 356b, 363
Times sign (×), use guidelines, 215
Titles (in references), See Article titles in
periodical citations, Book titles, Chapter
titles, Journal titles
Titles (in text)
abbreviation guidelines, 20, 150, 159, 160
artwork guidelines, 371, 377, 378
capitalization, 148–151, 227, 237t–239t
quotation marks use, 122
spelling recommendations, 127
standard format, 20
trademarks not used in, 157
unnumbered lists in manuscripts, 374
Titles (professional or personal)
in bylines, 21
capitalization, 147–148
foreign surnames, 152
“To”
capitalization in infinitives, 149
vs en dash, 124–125, 209
“To be” verb forms, 51, 111, 143
Toner cartridges for figure artwork, 353b, 360
Top-level elements (markup language compo-
nent), 91
“torr” vs “Torr”, 225
Toxic Substances Control Act Inventory, 254
Trade names vs generic names, 157
Trademark symbol, 23, 157
Trademarks
capitalization, 146, 157
definition, 157
scientific paper format, 23
in titles, 20
use guidelines, 157
“Trans”, italicization and capitalization, 145, 150
Transcripts of speeches, 57
Transfer of copyright, 32, 33, 78, 82, 86
Transitional phrases
comma use, 117
semicolon use, 119–120
Translations, citation formats, 299
Transliteration of foreign names, 153
Transport properties, 212, 215, 283
Transposes of matrices, 213
Tree view of markup languages, 94, 95f
“tri” in element names, 260
Tricky possessives and plurals, 127–128
Trigonometric and other functions
line breaks, 220
roman type use, 213, 220
spacing considerations, 213
Trim size for ACS books, 354f
Trigonal bonds in chemical formulas, 267
Tritium, representation, 264, 266
Trivial chemical names, 22
TrueType font format, 357b
Truncation in e-mail addresses, 157
Two-letter initials, foreign names, 153
Two-letter variables, italic type use, 212
Two-word compounds, hyphenation, 137, 138
See also Compound words
Two-word concepts, en dash use, 124–125
Two-word verbs, hyphenation, 139
Type and photograph combinations, See
Combos (artwork)
Type size
chemical reactions, 272
figures, 353b, 356b, 357b, 358f, 360, 365
structures, 378
tables, 373
Type weight, definition and examples, 356b
Typefaces, See Boldface type, Fonts, Italic type, Roman type
U for uniform labeling, 265
“U.K.” in references, 294, 303, 310
when to abbreviate, 161
Undergraduate students and peer review, 9, 75
Underscore in e-mail addresses, 157
Unhyphenated prefixes, 135–136
Uniform resource identifier (URI), 92
Uniform resource locator (URL)
in Internet reference citations, 315, 317–320
line break guidelines, 156
persistent URIs, 317
WWW address format, 156
WWW history, 89
See also World Wide Web sites
Unit cells, crystallographic types, 269
Unit modifiers
capitalization in titles and headings, 150,
225, 227
definition and types of, 139–140
editorial list, 140
foreign phrases as, 139
hyphenation, 138, 139–143
phrasal verbs as, 139
as predicate adjectives, 143
serial, with same ending base, 141
three or more words, 142–143
Unit of measure–number combination as
singular, 51
United Kingdom
in references, 294, 303, 310
when to abbreviate, 161
United States
commercial chemical inventories, 254
when to abbreviate, 161
See also U.S. entries
Units of measure
abbreviating vs spelling out, 160, 225–226
axis labels on illustrations, 359
capitalization, 150, 225, 227
case sensitivity, 159
as collective nouns, 107
comparison words, 51
compound, 224, 226, 230
decimals use, 208
definition not required, 224
discipline-specific preferences, 207
hyphenation of unit modifiers, 141–143
large numbers with, 207
non-SI units list, 231
not having abbreviations, 225
numeral and word usage, 203, 204
period use, 118, 223
plural forms, 224, 225
in ranges and series, 226
roman type use, 212
spacing, 203, 223–224, 271–272
spelling out, 160, 225–226
surnames as, 151–152, 225
systems overview, 228
in tables, 207, 225, 371, 373
usage overview, 223–227
See also SI units
Units of temperature
capitalization, 225
degree symbol guidelines, 203, 208, 224, 227
non-SI units list, 231
SI units list, 229
Units of time
decimals use, 208
hyphenation of unit modifiers, 141
minute and second symbol spacing, 203, 224
month abbreviations, 160–161
non-SI units list, 231
numeral and word usage, 160, 203, 205
roman type use, 212
seasons capitalization, 149
SI units list, 229
University name and location in thesis cita-
tion, 310
Unknown quantities
defining symbols in text, 211
italic type use, 212
Unnamed chemical elements, 260
Unprimed numbering, 244
Unpublished materials
ethical obligations
authors, 7
editors, 12–13
reviewers, 9, 16
reference format, 308–309, 315–316, 322
URI (uniform resource identifier), 92
URL, See Uniform resource locator
"U.S."
in references, 294
when to abbreviate, 161
U.S. Code, cited as reference, 313
U.S. Copyright Office, 79–80, 82
U.S. Department of Health and Human Ser-
vices, Office of Research Integrity, 4
U.S. government authorship, ACS copyright
policy, 81
U.S. Government Printing Office, 311, 312
U.S. government publications
cited as references, 292, 295, 311–313, 321
Code of Federal Regulations, 313
copyright, 81, 366
Federal Register, 313
U.S. Code, 313
U.S. Laws, 313
U.S. laws, cited as reference, 313
U.S. monetary values, 208
U.S. National Institute of Standards and Tech-
nology, 101
U.S. patents
cited as reference, 292, 310–311
style guidelines, 208
U.S. Postal Service abbreviations, 161–162,
303, 310
U.S. regulatory agencies, 254
"U.S.A.", CASSI spacing exception, 294
Usage of words, See Word usage
User names for author home pages, 62
Uuencoded files, 62
UV–visible spectroscopy, reporting analytical
data, 276
Valence configurations, 256
Validation of datuments, 96–97
Validation reports for CIF compliance, 63, 286
“Values” with plurals of symbols, 211
Vanadium symbol, avoiding confusion with
numerals, 262
Variables
in combinatorial chemistry, 246, 250
defining, 211, 225, 371
Greek letter use, 214
italic type use, 212
as mathematical concept, 210
roman type use, 213
spacing between, 215, 219
Variety names
capitalization, 146
italic type use, 154
“Variety of” as collective noun, 106
Vectors
boldface type for vectors, 213
Greek letter use, 214

Vectors—continued
italic type for components, 212
as mathematical concept, 210
Verb–subject agreement, 43–44, 105–108
Verb tenses, 42–43
Verbs, phrasal, 139, 150
Verbs, two-word, 139
“Versus”, 50, 124–125, 160
Video
still shot permissions, 83
Web-enhanced objects, 25, 26
Vietnamese surnames, 153
Vocabularies, controlled, 97–98
Voice, See Active voice, Passive voice
Volume number
books, 303–304, 306
meetings and conferences, 308
periodicals, 295, 296, 297–298
“vs”, 160
Water of hydration, centered dot use, 261
“We”, writing style, 43–44
Web-based applets for drawing, 379
Web-based publications
caption preparation, 365
font tips, 357b
illustration preparation, 344, 346, 350–352
reference accuracy, 24, 30, 31
supporting information, 25
See also Electronic source citation, Online
books, Online periodicals
Web-based search engines, 99, 383
Web-based systems
manuscript submission via, 31, 32, 59–69
permission requests via, 83–84
proof return via, 34b
reference management programs, 326–327
supporting information on, 5, 25
Web browsers
electronic submission of manuscripts, 61, 68
markup language display, 94
markup languages and the WWW, 90
Web-enhanced objects (WEOs), 25–26
Web sites, See World Wide Web sites
WebLab Viewer (helper application), 25
Webster’s New World College Dictionary, 127, 135
Webster’s Third New International Dictionary, 127, 135
“Well”, hyphenation in unit modifiers, 141
When to publish, See Timeliness as issue
“Whereas”, usage guidelines, 46
“Whether” vs “Whether or not”, 52–53
“Which”, with nonrestrictive clauses, 109
“While”, usage guidelines, 46
“Who”, with nonrestrictive clauses, 109
“wide”, hyphenation as suffix, 138
“Wife”, gender-neutral alternatives, 58
Windows platform
reference manager programs for, 327
templates for, 29
“With”, alternatives to, 56
Word (software), 61, 352, 363, 373, 379
Word choice, See Word usage
Word definitions, italic type use, 154
Word omissions
in comparisons, 48–49
verbs and auxiliary verbs, 108
Word order
in comparisons, 48–49
sentence construction, 45–46
Word-processing file formats, See Computer file formats
Word-processing software
electronic submission of manuscripts, 61
figure preparation, 352, 363
reference management programs, 326
structure preparation, 379
table preparation, 373–374
Word-processing templates, See Templates
Word spacing. See Spacing
Word usage
in captions, 365
confusable words and phrases, 51–53,
111–112
gender-neutral language, 57–58
grouping and comparison words, 50–51
and manuscript revisions, 32b
numeral and word usage, 160, 203–207
in scientific vs other writing, 16, 28, 50
in titles, 20
units of measure guidelines, 223–227
words and phrases to avoid, 54–57
Wordiness
in article titles, 20
examples, 54–55
WordPerfect (software), 61, 352, 363, 373
Works made for hire and copyright, 78, 82
World Wide Web
and markup languages, 89–96
URL forms, 136
World Wide Web sites
ACS author guidelines, 29, 343, 381b
ACS ethical guidelines, 11
ACS permission requests, 83
ACS publication home pages, 28b
ACS Publications Division, 86
ASAP articles, 34
author guidelines on, 75
Cambridge Crystallographic Data Centre, 284, 286
World Wide Web sites—continued
Chemical Abstracts Service, 253
citation of Internet sources, 293t, 314,
320–321
company sites, 127
computer and Internet terms on, 163–168
copyright issues, 79, 81, 82, 83
CRYSTMET database, 284
data set citation format, 314
DOI system, 317
drawing software resources on, 380, 380b
Dublin Core Schema, 90
electronic submission of manuscripts via,
60, 65t–67t
graphics resolution on, 364
ICSD database, 284
International Organization for Standardization,
255
International Union of Crystallography,
284, 286
International Union of Pure and Applied
Chemistry, 97, 102, 255, 383
molfile format information on, 381
National Academy of Sciences, 4
National Institute of Standards and Technology,
228, 255
Nucleic Acid Database, 284
Office of Research Integrity, 4
Organic Syntheses, 305
peer-review information, 71
Protein Data Bank, 284
STIX font downloads on, 357b
structure representation standards on, 383
supporting information on, 25
templates on, 29
XML-related information, 90
Year of publication
books, 303
diary, 302
dissertations, 309
periodicals, 296, 297–298
theses, 310
U.S. government publications, 312
See also Author–date citations
“Yet” as coordinating conjunction, 47, 113,
149
Z prefix in chemical names, 236
Zero
before decimal point, 208
as electric charge indicator, 256
Zipped files, 62
Writing style—continued
usage guidelines, 50–58, 111–112, 160,
203–207, 223–227
See also specific aspects
WWW, See World Wide Web entries
X for products mixed, 246, 251, 252
“X-ray”, capitalization, 144, 149
X-ray diffraction spectroscopy, reporting analy-
tical data, 276
XML (extensible markup language)
datument as scientific grid component, 99
datument potential, 99
datument validation, 96
datument vocabularies, 98
display of, 94–96
elements of, 90–94, 91s
WWW history, 90
XML Query protocol, 99
Xpress Track (software), 60
XSL (extensible stylesheet language), 90
XSLT technology, 94
Zones, crystallographic notation, 268