

## Notice to Authors of JACS Manuscripts

(Revised January 2016)

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### **Important Manuscript Submission Requirements and Notices**

- When a manuscript is submitted to JACS, Editors must make an initial editorial judgment regarding its suitability for the journal’s audience. A significant number of submissions are returned without sending them on for further processing.
- Titles of manuscripts may not contain the words “First” or “Novel” nor any part number or series number.
- The use of acronyms in titles, unless common, is strongly discouraged.
- Title of manuscript, list of authors, and order of authors must be the same on all pieces of the submission.
- All authors must be listed on the submission page with current contact information and a direct/valid e-mail address for each.
- Communications and Articles must contain both an Abstract and a Table of Contents (TOC) graphic in the manuscript document file.
- Communications must be prepared in the current [Communications template](#) and may not exceed 4 pages.
- All sections of an Article must be properly labeled (Introduction, Discussion, Experimental Section, Conclusions, etc.).
- Turn “track changes” off before submitting files; upload annotated files as Supporting Information for Review Only.
- Copies of all related works that are “in press”, “accepted”, or “submitted” for publication or in the late stages of preparation must be uploaded as Supporting Information for Review Only at the time of submission. References that are only available online should be cited by the Digital Object Identifier (DOI).
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- Crystallographic information files must be furnished for all new structures, even if they have already been submitted to the CCDC, ICSD, or PDB. They must be submitted in CIF format and uploaded as Supporting Information for Publication.
- Dedications may appear only in the Acknowledgment section and are subject to approval by the Editor.
- The receipt date will be recorded as the date the complete manuscript is received by the Editor’s office. Manuscripts that are ready to be reviewed when first submitted will receive priority for initial processing and assignment to an Associate Editor.

- The publication date will be recorded as the date the paper first appears online as an ACS Publications product—the earliest of “Just Accepted”, “Articles ASAP”, or issue publication date.
- A Journal Publishing Agreement is required for publication. Authors are strongly encouraged to use the Electronic Journal Publishing Agreement. If the PDF version is used, all pages of the signed Agreement must be uploaded in TIF or PDF format to the ACS Paragon Plus Environment or e-mailed, faxed, or mailed to the assigned Associate Editor.
- Failure to adhere to one or more of the ACS [Ethical Guidelines to Publication of Chemical Research](#) will result in disciplinary action.

## Scope and Editorial Policy

The *Journal of the American Chemical Society* is published weekly and is devoted to the publication of fundamental research papers in all fields of chemistry. Articles, Communications, Perspectives, and Spotlights are published. “Notes” and “Comments” on earlier work are not considered or published.

**Initial Editorial Review.** *JACS* is devoted to the publication of original, fundamental research of unusual urgency and significance in all fields of chemistry that appeals to a broad, general audience. Competition for publication within *JACS* is intense, and the journal is simply unable to publish all the sound work received. When a manuscript is submitted to *JACS*, Editors must make an initial editorial judgment regarding its suitability for the journal’s multidisciplinary readership. Submissions that, in the judgment of the Editors, are outside the journal’s scope or are not sufficiently novel are returned without sending them on for further processing. This procedure helps ensure that the many worthwhile manuscripts containing specialized work may be submitted elsewhere without undue delay.

**Manuscript Submission.** Manuscripts must be submitted via the [ACS Paragon Plus Environment](#). *JACS* does not accept mailed, faxed, or e-mailed submissions. Complete instructions, an overview of the Web submission process, and online support are available through the secure ACS Paragon Plus Web site.

Submission of a manuscript to *JACS* is contingent upon the agreement by all the authors that the reported work has not received prior publication and that no portion of this or any other closely related work is under consideration for publication elsewhere in any medium, including electronic journals, computer databases, and publicly accessible preprint Web sites. Authors must adhere to the American Chemical Society’s [Ethical Guidelines to Publication of Chemical Research](#), which are available on the Web. Failure to adhere to one or more of the ethical guidelines will result in disciplinary action.

Manuscripts submitted to *JACS* should be written in a style that addresses a wider audience than for papers prepared for more specialized journals. Authors should present their materials with the utmost conciseness and clarity. Articles that exceed the norm of 8-10 Journal pages often contain a level of detail that is not appropriate for a broad audience. Manuscripts exceeding this length may be returned to the authors for shortening prior to review.

**Articles** most appropriate for publication in *JACS* are those that deal with some phase of “pure” chemistry as distinguished from “applied” chemistry. Because of restrictions on the number of published pages in the Journal, not all manuscripts that describe well-executed work can be accepted. Articles of high scientific quality, originality, significance, and conceptual novelty that are of interest to the wide and diverse contemporary readership of *JACS* will be given priority for

publication. Articles on methodology should include one or more applications of widespread interest and, unless significant new advances are announced, will be declined with the recommendation for submission to specialized journals. Papers that draw conclusions from the treatment of existing data must also include significant new data and make new experimental or theoretical predictions of broad interest. Articles which mainly expand findings that were previously published as Communications in *JACS* or elsewhere and which only incorporate experimental data, without greatly expanded scope and without providing new insights or conceptual breakthroughs, will be declined. Articles that are mainly routine extensions of previously published related work will also be declined with the recommendation for submission to more specialized journals.

**Communications** are restricted to reports of unusual urgency, timeliness, significance, and broad interest. A brief statement explaining how the manuscript meets the criteria of urgency and significance should be included in the author's cover letter. It is desirable that the principal conclusions be stated in the opening sentences of the manuscript. Communications of up to 4 Journal pages will be considered. The submission of multiple Communications on the same or closely related topics within a short period of time is not an acceptable means of publishing a body of work that is too large for a single Communication. Such work should be described in the format of an Article. The major concepts must not have appeared previously as a report or publication (e.g., published lecture or news release, electronic journal paper or preprint, symposium proceedings, or an extended abstract such as *Polymer Preprints*). If a previous Communication by the same author(s) has already appeared and the present manuscript describes a technical improvement or increase in the scope of the work, it will not be accepted in the absence of a novel conceptual advance.

**Perspectives** are personal reviews of a field or area, and they are focused rather than comprehensive. Perspective authors are asked to assess the current status of the field with an emphasis toward identifying key advances being made or those advances that are needed, and with an eye to the future. The *JACS* Perspective should touch base with the current literature, including key contributors and references, but will primarily serve to inspire and help direct future research efforts. Authors may be invited by the Editor to submit Perspectives. Authors interested in submitting a Perspective are strongly encouraged to contact the Editor prior to manuscript preparation and submission, to seek conditional approval of the proposed topic. One-page proposals should be sent to the Editor, Peter J. Stang ([jacs@jacs.acs.org](mailto:jacs@jacs.acs.org)), for consideration. Perspectives should be in the range of 5-10 formatted Journal pages.

**Additions and Corrections** may be used to address important issues or correct errors and omissions of consequence that arise after publication of an article. Additions and Corrections may be requested by the author(s) or initiated by the Editor after discussions with the corresponding author. Readers who detect errors of consequence in the work of others should contact the corresponding author of that work. All Additions and Corrections are subject to approval by the Editor, and minor corrections and additions will not be published. Additions and Corrections from authors should be submitted via the [ACS Paragon Plus Environment](#) by the corresponding author for publication in the "Addition/Correction" section of the Journal. The corresponding author should obtain approval from all of the article coauthors prior to submitting an Addition and Correction, or provide evidence that such approval has been solicited. The Addition and Correction should include the original article title and author list, citation including DOI, and details of the correction. For proper formatting, see examples in a current issue of the Journal.

**Retractions.** Articles may be retracted for scientific or ethical reasons. Articles that contain seriously flawed or erroneous data such that their findings and conclusions cannot be relied upon may be retracted in order to correct the scientific record. Retractions may be requested by the article author(s) or by the journal Editor(s), but are ultimately published at the discretion of the Editor. When an article is retracted, a notice of Retraction will be published containing information about the original article title, author list, and the reason for the Retraction. Retracted articles will be accompanied by the related Retraction notice and will be marked as “Retracted”. The originally published article will remain on the web except in extraordinary circumstances (e.g. where deemed legally necessary, or if the availability of the published content poses public health risks). The American Chemical Society follows guidance from the Committee on Publication Ethics (COPE) when considering retractions; for more information see <http://publicationethics.org/>.

**Supporting Information.** Sufficient experimental or computational information must be deposited in the Supporting Information to enable readers to reproduce the authors’ results (see the ‘[Supporting Information](#)’ section under Preparation and Submission of Manuscripts). The Supporting Information should include selected experimental and characterization data for key new compounds.

**Back-to-Back Publication.** Manuscripts intended for back-to-back publication will be considered. These manuscripts will be judged independently on their individual merit to ensure that they meet the qualifications outlined herein and that back-to-back presentation actually enhances the pedagogy and impact of the work.

**Computational Manuscripts.** For computational manuscripts to be suitable for publication in JACS, in addition to meeting the general requirements specified above for all Articles, it is required that (a) the level of theory and methodology employed must be adequate for the problem at hand, and (b) the manuscript must provide significant chemical insights or have substantial predictive value.

**Presubmission Inquiries.** Inquiries regarding the suitability of an abstract or manuscript for JACS will not be considered prior to submission of the complete manuscript file through the ACS Paragon Plus Environment.

**Incomplete Manuscripts.** Manuscripts that are incomplete at the time of submission must be revised to include the missing items or corrected files before peer review. The official date of receipt of the manuscript will be recorded as the date that the revised manuscript is received in the Editor’s office in the complete and proper format.

**Plagiarism.** Manuscripts must be original with respect to concept, content, and writing. It is not appropriate for an author to reuse wording from other publications, including one’s own previous publications, whether or not that publication is cited.

**Related Work by Author.** All related work under consideration for publication in any medium must be cited in the manuscript, and the Editor must be informed at the time of submission. When related work by any of the authors is not available because it is in press (accepted), submitted, or in preparation for submission to JACS or another journal, a copy of each related paper should be uploaded as “Supporting Information for Review Only” at the time of submission. If a cited reference has already appeared on the Web, indicate that it is published

electronically (“Just Accepted” or “ASAP” for ACS journals) and give the DOI number for convenient access. The full journal citation should be completed during manuscript revision or page proof correction, if possible.

**Peer Review.** The Editors generally seek the advice of experts about manuscripts; however, manuscripts considered by the Editors to be inappropriate for *JACS* may be declined without review. The recommendations of reviewers are advisory to the Editors, who accept full responsibility for decisions about manuscripts. Final responsibility for acceptance or declination rests with the Editor.

Authors are urged to suggest in the cover letter a minimum of six to eight persons competent to review the manuscript, at least half of whom must be from North America. Authors may also request that specific people not be used as referees, and they may include reasons for such a request. These suggestions will be advisory to the editors and are not a condition for submission. Reviewer identities are confidential, and the names of reviewers will not be revealed to an author.

Reviewers are asked to evaluate manuscripts on the scientific value of the work, the level of interest to the broad and diverse readership, the appropriateness of the literature citations, and the clarity and conciseness of the writing.

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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." Deletion of an author after the manuscript has been submitted requires a confirming letter to the Editor-in-Chief from the author whose name is being deleted. For more information on ethical responsibilities of authors, see the [Ethical Guidelines to Publication of Chemical Research](#).

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**Embargo on Release of Information Prior to Publication.** Authors must use care in the disclosure of scientific results and conclusions contained in a *JACS* manuscript before the manuscript is published on the *JACS* "Just Accepted Manuscripts" or "Articles ASAP" Web site. Publication of these results and conclusions in the public domain (popular press, press release, preprint server, or other outlet) constitutes prior publication. As a result, the manuscript may be immediately withdrawn from *JACS* and will not be published.

**Revised Manuscripts.** When a revision is requested after peer review, the authors must return the revised manuscript promptly: 14 days is allotted for minor revisions of both Articles and Communications, 30 days for major revisions of Articles, and 21 days for major revisions of Communications. After the allotted time, a revised manuscript will be handled as a new submission and will be given a new receipt date.

**Manuscript Transfer Service.** Occasionally editors in ACS Journals feel that manuscripts are a better fit for another ACS Journal and suggest that authors consider transferring the submission. The Manuscript Transfer Service simplifies and shortens manuscript submission to another ACS journal, as all the coauthors, suggested reviewers, manuscript files, and responses to submission questions are copied to the new submission. Once authors have selected a new journal, the journal office will facilitate the transfer to that journal.

To determine if a manuscript transfer is an appropriate next step, authors are encouraged to read "[Is Manuscript Transfer Right for Me?](#)" Authors are also reminded to review [journal editorial scope statements](#) as they consider the next destination for the submission.

Requirements of the new journal may be different, so authors should also check the Author Guidelines and make any needed revisions in order to conform to those requirements. Note that transferring a manuscript is not a guarantee that the manuscript will be accepted, as the final publication decision will belong to the editor in the next journal. Please keep in mind that the reviews, reviewer identities, and decision letter will all be transferred to the new journal. For complete details, see [http://pubs.acs.org/page/policy/manuscript\\_transfer/index.html](http://pubs.acs.org/page/policy/manuscript_transfer/index.html).

**Resubmission to JACS.** The resubmission of manuscripts previously considered and declined for publication in *JACS* is strongly discouraged and will only be considered under extraordinary circumstances.

**Well-reasoned appeals of decisions may be considered, but must first be directed to the Associate Editor who handled the original submission and not to the Editor.**

**If a paper has been declined by JACS and the author wishes to submit a revised version, the author is required to first gain consent from the Associate Editor who handled the initial submission.** If the Associate Editor's consent to resubmit is received (which does not guarantee ultimate acceptance), the cover letter must explicitly state that permission was obtained from the Associate Editor and must describe the changes that have been made in the manuscript and include justification for reconsideration. The manuscript will be assigned to the same Associate Editor who handled the initial submission. The request for reconsideration may be denied without further review if, in the Editor's opinion, no adequate new science was provided or the work is more suitable for publication in a specialized journal.

**Publication Date.** Manuscripts accepted for publication in ACS journals are published online rapidly, whereupon they may be cited by reference to the unique Digital Object Identifier (DOI) that is assigned to each manuscript. The publication date is recorded as the date a paper first appears online as an ACS Publications product—the earliest of “Just Accepted”, “Articles ASAP”, or issue publication. Once published online, a manuscript may not be temporarily or permanently deleted from the Web. Authors should take this schedule into account when planning intellectual and patent activities related to a manuscript. The actual date on which an accepted paper is published on the Web is recorded on the Web version of the manuscript and on the first page of the PDF version.

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It is the responsibility of the corresponding author to ensure that all authors listed on the manuscript agree with the changes made on the proofs. Comments on the proofs should be returned within 48 hours of receipt to ensure timely publication of the manuscript.

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# Preparation and Submission of Manuscripts

## Journal Publishing Agreement

A properly completed and signed Journal Publishing Agreement must be submitted for each manuscript. ACS Paragon Plus provides an electronic version of the Agreement that will be available on the **My Authoring Activity** tab of the Corresponding Author's Home page once the manuscript has been assigned to an Editor. A PDF version of the Agreement is also available, but **authors are strongly encouraged to use the electronic Journal Publishing Agreement**. If the PDF version is used, **all pages of the signed PDF Agreement must be submitted**. If the Corresponding Author cannot or should not complete either the electronic or PDF version for any reason, another author should complete and sign the PDF version of the form. Forms and complete instructions are available at <http://pubs.acs.org/page/copyright/journals/index.html>.

## Cover Letter

A cover letter must be submitted at the same time as the manuscript. The cover letter may be created as a Word or PDF file or may be typed into the appropriate text box in the ACS Paragon Plus Environment. The letter must provide the corresponding author's name, postal and e-mail addresses, and telephone and fax numbers. All Editorial correspondence concerning receipt, status, review, revision, and publication of a manuscript will be sent only to one person who has been designated as the corresponding author during the evaluation period. The corresponding author is responsible for communicating the manuscript status to all coauthors of the paper and for obtaining the coauthors' assent to any substantial changes of content or interpretation made during revision. The cover letter may suggest the name of an appropriate *JACS* Associate Editor. However, manuscript assignment to an Associate Editor is ultimately at the discretion of the Editor. Authors must suggest a minimum of six to eight persons competent to review their manuscript, at least half of whom must be from North America. The selection of appropriate reviewers is the prerogative of the Associate Editor handling the manuscript.

The cover letter should provide explicit assurance that the manuscript is not under consideration for publication and has not been published elsewhere in any medium including electronic journals and computer databases of a public nature.

## Manuscript Submission

All manuscripts must be submitted through the [ACS Paragon Plus Environment](#). Complete instructions and an overview of the Web submission process are available through the secure ACS Paragon Plus Web site. Authors must also submit all revisions of manuscripts via the ACS Paragon Plus Environment. The Web submission site employs state-of-the-art security mechanisms to ensure that all electronically submitted papers are secure. These same security mechanisms are also utilized throughout the peer-review process, permitting access only to editors and reviewers who are assigned to a particular paper.

## Preparation of Manuscripts

**Communications.** Authors who submit Communications are required to use the current [Communications template](#) available from the submission Web site. Use of the word-processing

template will ensure proper formatting and will facilitate review. It will allow authors and Editors to estimate the publication length of Communications at submission. Authors will be required to modify Communications that exceed the four-page limit at the page proof stage.

All graphics and tables must be placed in the Communication template near the point of first mention in the text of the manuscript (not grouped at the end of the document).

**Articles.** Use of the template for Articles is strongly encouraged but is not required (use of the template for Communications is mandatory). If an author chooses not to use a template to prepare an Article, only Times and Symbol fonts and 1.5 or double line spacing should be used. Other fonts may cause problems when the PDF files used for review are created. Also, if the template is not used, the document mode or its equivalent in the word-processing program should be used; i.e., files should not be saved in “Text Only” (ASCII) mode. If a non-Western version of word-processing software is used to prepare the manuscript, the file should be saved in rich-text format (RTF).

Graphics and tables must be placed within the Article manuscript file near the point of first mention in the text.

**General Considerations.** All files must be saved with U.S. Letter page-size (in the Page Setup settings of the word-processing application) before submission on the Web. Authors should consult recent issues of the Journal and [\*The ACS Style Guide\*](#), 3rd ed.; American Chemical Society: Washington, DC, 2006, for further format guidance.

Authors are required to provide a word processing file of their manuscript. Authors may provide their own manuscript PDF file along with the manuscript file or provide the manuscript file only and allow ACS to convert it to PDF. When creating the PDF files for submission (required for the manuscript and cover letter if they are furnished in a file type other than Microsoft Word), it is essential that all fonts be embedded within the PDF file. All characters must be correctly represented throughout the manuscript: for example, 1 (one) and l (ell), 0 (zero) and O (oh), x (ex) and  $\times$  (times sign), and ' (prime) and ’ (apostrophe). The Symbol font should be used for all Greek letters and math symbols.

Any author who is not fully fluent in idiomatic English is urged to obtain assistance with manuscript preparation from a fluent colleague or through a paid editing service. Manuscripts with grammar or language usage deficiencies are handicapped during the scientific review process and may be returned to the author for rewriting before peer review or before acceptance.

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information on submitting TeX/LaTeX files, see [Preparing and Submitting Manuscripts Using TeX/LaTeX](#).

**Table of Contents Graphic.** The Journal features a Table of Contents (TOC) that contains a graphic presentation for each Communication and Article entry, in addition to the title and author list. Authors are required to submit a graphic for the TOC that, in conjunction with the manuscript title, is meant to convey to the reader the essence of the work and thereby capture the reader's attention. It may be a key structure, reaction, equation, concept, or theorem, etc., or an ingenious representation thereof, that is discussed in the manuscript. The use of color to enhance the visual appeal of the TOC graphic is encouraged. The TOC graphic must appear on the last page of the Communication or Article manuscript file.

See the '[Artwork](#)' section for instructions for preparing the TOC graphic. Authors are encouraged to examine the Table of Contents in a current issue for appropriate examples, or visit the [JACS Web site](#). The TOC graphic is subject to approval by the Editor.

**Title.** The title should accurately, clearly, and concisely reflect the emphasis and content of the paper. Series or part numbers may not be used, nor may the words "Novel" or "First" appear in the title. Acronyms and abbreviations are not permitted in manuscript titles, unless they are broadly familiar to readers in all disciplines of chemistry.

**Author List.** Include as coauthors all those who have made substantial contributions to the work. Use first names, initials, and surnames (e.g., John R. Smith). Do not use only initials with surnames (e.g., J. R. Smith), because this causes indexing and retrieval difficulties and interferes with unique identification of an author. Deceased persons who meet the criteria for inclusion as coauthors should be so included, with an Author Information note indicating the date of death. Do not include professional or official titles or academic degrees. At least one, or optionally more than one author must be designated with an asterisk as the author(s) to whom reader correspondence regarding the published manuscript may be addressed.

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**Institution Address.** The author affiliation(s) listed should be the institution(s) where the work was conducted. If the present address of an author differs from that at which the work was done, that address should be given in an Author Information note.

**Abstract.** All manuscripts (Communications and Articles) must contain an abstract, which should summarize the reason for the work, the most significant results, and the conclusions. The abstract should not exceed about 250 words. Pasting the abstract in the text box on the Web submission page does not replace the need for including an abstract in the manuscript document.

**Text (Articles).** The first paragraphs of an Article should explain the motivation for and import of the work, where it fits in the development of the field and of chemistry, and perhaps why it should be of interest to chemists in other areas. It should be possible to do this without excessively increasing the length of the Article. Extensive reviews of the literature cannot be

accepted. Thoughtful use of schemes and figures (with well-composed captions) is recommended, so that even casual browsers can discern the nature of the work. Well-known procedures should be designated by name, or literature references to them should be given. Experimental results are of lasting value and should be clearly and logically presented in a separate section. Standard Article format must be used for preparing a manuscript for submission as an Article, including section headings and a proper Introduction, a complete Experimental Section (unless placed in the Supporting Information), Results, and Discussion. The addition of a Conclusion section at the end of the paper, which briefly summarizes the principal conclusions of the work, is recommended. If desired for clarification, section headings may be given Arabic numbers and subsections numbered in decimals (e.g., subsection 2.1 and subsection 2.2).

**Text (Communications).** Section headings (Introduction, Experimental Section, Conclusion, etc.) should not be used in a Communication.

**Self-Citations.** The use of excessive self-citations is not permitted.

**Disclaimers.** Disclaimers are not allowed in *JACS* manuscripts or in the Supporting Information.

**Appendices.** Appendix sections must be placed in the Supporting Information.

**Dedications.** All dedications must appear in the Acknowledgment section and are subject to approval by the Editor.

**Abbreviations.** Acronyms and abbreviations that are not broadly familiar to readers in all disciplines of chemistry should be introduced in parentheses following the full term on its first appearance in the text. Do not include a separate Abbreviations list.

**Acknowledgment.** Dedications and notes acknowledging financial or professional assistance to the conduct of research or indicating presentation at a meeting should be brief and placed in the Acknowledgment section.

**Author Information Notes.** The e-mail address(es) of the corresponding author or authors must be provided as a Corresponding Author note. Present addresses for individual authors that differ from the address(es) at which the work was done should be given in a Present Addresses note.

Simple equal authorship statements are allowed and may be presented in an Author Contribution note. However, itemization of individual author contributions or partial authorship is not permitted in any part of the manuscript or Supporting Information.

**Associated Content.** A brief statement in non-sentence format must be included at the end of the manuscript, which describes any material placed in Supporting Information and the means by which the interested reader may obtain it. The following format should be used:

**Supporting Information.** Brief statement in nonsentence format listing the contents of the material supplied as Supporting Information.



A description of any Web Enhanced Objects (WEOs) must also be provided, in the following format:

**Web Enhanced.** A WEO is available in the HTML version of the paper.

For instructions on what material should be provided as ‘[Supporting Information](#)’ or ‘[Web Enhanced Objects](#)’ and on preparing it for publication, see the respective section below.

**Figures.** Figures must include a caption giving the figure number and a brief description, preferably only one or two sentences. The caption should be understandable without reference to the text. It is preferable to place any key to symbols used in the artwork itself, not in the caption; colored symbols cannot be reproduced in the caption. Ensure that any symbols and abbreviations used in the text agree with those in the artwork.

**Schemes.** Sequences of reactions are called schemes. Schemes may have brief titles describing their contents and footnotes, if needed, for further detail.

**Charts.** Groups of structures that do not show reactions are called charts. Charts may have brief titles describing their contents and footnotes, if needed, for further detail.

**Tables.** Tables should be used when the data cannot be presented clearly as narrative, when many numbers must be presented, or when more meaningful interrelationships can be conveyed by the tabular format. Tables should supplement, not duplicate, information presented in the text and figures. Tables should be simple and concise. Each table must have a brief (one phrase or sentence) title that describes the contents. The title should be understandable without reference to the text. Details should be put in footnotes, not in the title. Define nonstandard abbreviations in footnotes. Footnotes in tables should be given letter designations and be cited in the table by italic superscript letters. The sequence of letters should proceed by line rather than by column. If a reference is cited both in the text and in a table, a lettered footnote that refers to the numbered reference in the text should be placed in the table.

Tables may be created using a word-processor’s text mode or table format feature. The table format feature is preferred. Ensure that each data entry is in its own table cell. If the text mode is used, separate columns with a single tab and use a line feed (return) at the end of each row. In setting up tables, authors should keep in mind the type area of the *JACS* and should make tables conform to the limitations of these dimensions.

All **Figures**, **Schemes**, **Charts**, and **Tables** should be rendered legibly (please see the ‘[Artwork](#)’ section for requirements) and must be mentioned in the text in consecutive order. Figures, Schemes, Charts, and Tables must be numbered consecutively with Arabic numerals and placed in the document within the text near the point of first mention.

**Web Enhanced Objects.** The editors of the *Journal of the American Chemical Society* encourage the submission of Web enhanced objects (WEOs) that complement a reader’s understanding of the research being reported. These types of files include color figures (including 3D rotatable figures), animations, spectra, video, and sound. Links to WEOs will appear in the Web HTML edition of the paper. Files suitable for this form of publication should be viewable with commonly available Internet plug-ins or helper applications. More information on [Specifications for Web Enhanced Objects](#) is available on the Web. Authors should submit

WEOs via the Paragon Plus Web site as part of their submissions, using the file type designation “Web Enhanced Object”. Descriptions of WEOs should be included in the appropriate places within the related graphic caption or text of the paper and summarized in the Associated Content section, noting the type of file and format. Example: “A 3D rotatable image in xyz format is available.”

**References and Footnotes.** *All the references and footnotes must be placed together in a list at the end of the manuscript text.* In the Web edition, many of them will have links to other Web resources, such as the corresponding abstracts in *Chemical Abstracts* and the full text on publisher Web sites. Because of this electronic linking, and to aid scientific research, *it is crucial that authors verify the accuracy of all reference citations and footnotes.*

Unnecessarily long lists of references should be avoided, and excessive self-citation is not permitted. However, authors must reference all previous publications in which portions of the present work have appeared. Literature references and explanatory footnotes must be numbered with Arabic numerals in the order of their first citation in the text and the corresponding numbers placed at the appropriate locations in the text as superscripted numerals.

Long footnotes should be avoided; additional data and peripheral discussion should be placed in the Supporting Information rather than in footnotes. Supplementary references may be placed in Supporting Information.

Bibliographic references to classified documents and reports or references to unpublished materials that are not generally available to the scientific public should not be used. Authors must obtain written permission from any person whose work is cited as a personal communication, unpublished work, or work in press. Copies of letters of permission and documentation should be appended to the cover letter file. If the manuscript is accepted but the necessary permissions have not been received, the Editor will ask the author to remove the reference(s) and dependent text.

Authors should consult [The ACS Style Guide](#), 3rd ed.; American Chemical Society: Washington, DC, 2006, for the appropriate style to use in citations of journal papers, books, and other publications. In literature references, journal abbreviations should be those used in the [Chemical Abstracts Service Source Index \(CASSI\)](#).

**Nomenclature.** Registered trademark names should be capitalized whenever used. Trade and trivial names should not be capitalized. It is not necessary to use the trademark, registered trademark, or service mark symbol to ensure legal protection for the trademark.

## Artwork

**General Considerations.** Submission of graphics (illustrations) that are to be considered for publication in color is strongly encouraged. Color may be used to enhance the clarity of complex structures, figures, spectra, schemes, etc., and color reproduction of graphics is provided at no cost to the author. Graphics intended to appear in black and white or grayscale should not be submitted in color.

To facilitate the publication process, the preferred submission procedure is to embed (paste) graphic files into the manuscript Word document near the point of first mention. Most graphic

programs provide an option for changing the resolution (see below) when you are saving the image in the chosen file format. Best practice is to save the graphic file at the final resolution and size using the program used to create the graphic and then paste the graphic into the manuscript document. It may help to print the manuscript on a laser printer to ensure all artwork is clear and legible.

Individual graphics files, created by the author according to the following guidelines, may be uploaded to the ACS Paragon Plus Environment with the submitted manuscript.

**File Specifications.** Acceptable file formats are TIFF, PDF, EPS (vector artwork), or CDX (ChemDraw file). When submitting individual graphics, name the files based on graphic function (i.e., Scheme1, Figure2, Chart3, eq4, compd5), not the scientific name. Labels for multi-part figures should be present, and the parts should be assembled into a single graphic.

For TIFF files (either embedded in a Word document or submitted as individual files), the resolution requirements are as follow:

- black & white line art: 1200 dpi
- grayscale art (a monochromatic image containing shades of gray): 600 dpi
- color art (RGB color mode): 300 dpi

The RGB color mode and resolution requirements are essential for producing high-quality graphics within the published manuscript. Graphics submitted in CMYK or at lower resolutions may be used; however, the colors may not be consistent and graphics of poor quality may not be able to be improved. Graphics submitted at higher resolutions will be reduced to the resolution specified for the type of art as listed above.

For EPS files, ensure that all fonts are converted to outlines or embedded in the graphic file. The document settings should be in RGB mode. **NOTE:** *While EPS files are accepted, the vector-based graphics will be rasterized for production.*

Chemical structures should be produced with the use of a drawing program such as ChemDraw.

**Size.** Graphics should be submitted at the final publication size. Single-column graphics are preferred and can be sized up to 240 points wide (3.33 in.). Double-column graphics must be sized between 300 and 504 points (4.167 in. and 7 in.). The maximum depth for all graphics is 660 points (9.167 in.) including the caption (please allow 12 pts for each line of caption text).

Consistent sizing of letters, numbers, and labels in graphics throughout the manuscript will help ensure uniform graphic presentation for publication. Lettering should be no smaller than 4.5 points. Helvetica or Arial fonts work well for lettering. Lines should be no thinner than 0.5 point.

Note that all graphics are subject to approval by the Editor.

**Table of Contents (TOC) and Abstract Graphics.** A graphic should be submitted for use on the TOC; the same graphic may also appear along with the abstract. This graphic should give the reader a quick visual representation of the essence of the paper without providing specific details. The best images for these uses are simple and relatively free of text and technical

characters, and the use of color for visual impact is encouraged. Copyrighted images or TOC graphics that are not made by the author(s) should be avoided.

*Additional TOC Guidelines:*

- The graphic should uphold the standards of a scholarly, professional publication.
- The graphic must be entirely original, unpublished artwork created by one of the coauthors.
- The graphic should not include a photograph, drawing or caricature of any person, living or deceased.
- Do not include postage stamps or currency from any country, or trademarked items (company or institutional logos, images, and products).
- TOC graphics are subject to approval by the Editor.

**Cover Art.** JACS will feature a different image on the cover of each issue, and images chosen for the cover will be printed at no cost to the author. After favorable review, authors are invited to submit artwork suitable for consideration as a cover graphic. Cover art should be colorful and eye-catching and must convey the importance and significance of the research. Graphics in EPS, TIFF, JPEG, or PNG format (not PDF) should be 7.4 inches wide and 8.1 inches high, with a minimum resolution of 300 dpi (2100 × 2400 pixels), and submission of “layered” artwork is encouraged. Cover art files, as well as a short (<50-word), clear caption explaining the image, may be uploaded to ACS Paragon Plus as “Supporting Information for Review Only” during the final revision process. Upon manuscript acceptance, request for cover art should be sent directly to the Editor, Peter J. Stang ([jacs@jacs.acs.org](mailto:jacs@jacs.acs.org)), for consideration. Submitted images are evaluated and final selection is made by the Editor. These images may be modified or enhanced by an ACS graphic artist. Cover art may delay issue publication of the associated Article or Communication; however, ASAP publication will not be delayed.

For more information on working with graphics, please visit  
[http://pubs.acs.org/page/4authors/submission/graphics\\_prep.html](http://pubs.acs.org/page/4authors/submission/graphics_prep.html).

## Compound Characterization and Computational Data

**Characterization of New Substances.** Adequate evidence to firmly establish both identity and purity should be provided. Recommended criteria vary according to substance categories. A summary of the detailed criteria may be found on the Web in the JACS [Information for Authors](#).

**Spectra.** Reproductions of spectra, or the relevant segments thereof, will be published only if concise numerical summaries are inadequate for the purposes of the paper. Papers dealing primarily with interpretation of spectra and those in which band shape or fine structure needs to be illustrated may be published with such spectra included. Spectra will not be published merely as adjuncts to the characterization of compounds, however. See ‘[Supporting Information](#)’ below. Routine infrared, electronic, NMR, and mass spectra of new compounds should be numerically summarized, as appropriate, in the Experimental Section of an Article or in the Supporting Information of a Communication.

**Kinetic and Equilibrium Data.** For publication in the *Journal of the American Chemical Society*, the reporting of kinetic data and equilibrium binding data for proteins, nucleic acids, and

other species should preferably include a description of the identity of the catalyst or binding molecule, its origin, purity of composition, and any modifications such as mutations, post-translational modifications, or other modifications made to facilitate expression and purification. The method of assay and the exact experimental conditions of the assay should be provided as a reference to previous work, with or without modifications, or fully described if a new assay. Conditions essential to reproduce the results such as the temperature, pH, and pressure (if other than atmospheric) of the assay should be included. Terms such as “not detectable” (ND) should be avoided. Instead, an estimate of the limit of detection based on the sensitivity and error analysis of the assay should be provided. Authors are referred to the STRENDa (Standards for Reporting Enzymology Data) Commission of the Beilstein Institut (<http://www.beilstein-institut.de/en/projects/strenda/guidelines>) for an example of detailed guidelines.

**Reporting and Stewardship of NMR Data.** New guidelines recommend a standard baseline for the submission of NMR data to ACS journals. They are intended to promote accuracy and consistency. The guidelines are divided into three sections: NMR text, which outlines the preferred format for NMR data included in the Experimental Section; NMR spectra, which outlines the preferred format for inclusion of hard copies of spectra in the Supporting Information; and primary NMR data files, which outlines the procedure for submitting FID files, acquisition data, and processing parameters to include in the Supporting Information. Authors are strongly encouraged to provide all three sets of data for all new and/or key compounds described in a manuscript submission.

In the Experimental Section, the compound must be clearly identified, for example in a header at the beginning of the synthetic procedure or the summary of spectroscopic data. List the nucleus being measured, any nucleus being broad-band decoupled, the solvent used (formula preferred, e.g. C<sub>6</sub>D<sub>6</sub> over benzene-*d*<sub>6</sub>), the standard used, and the field strength. Field strength should be noted for each spectrum, not as a comment in the general Experimental Section. The standard(s) may be specified in the general experimental section; as an example, <sup>1</sup>H NMR data recorded in C<sub>6</sub>D<sub>6</sub> listed as “residual internal C<sub>6</sub>D<sub>5</sub>H (δ 7.15)”. Indicate solvent or peak suppression protocols used in collecting data. List the probe temperature when it is accurately known; ambient probe temperature is otherwise understood. Give <sup>1</sup>H NMR chemical shifts to two digits after the decimal point. Include the number of protons represented by the signal, peak multiplicity, and coupling constants as needed (*J* italicized, reported with up to one digit after the decimal). The number of bonds through which the coupling is operative, <sup>x</sup>*J*, may be specified by the author if known with a high degree of certainty. Accepted abbreviations for multiplicities and descriptors are s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, m = multiplet (denotes complex pattern), dd = doublet of doublets, dt = doublet of triplets, td = triplet of doublets, and br = broad signal.

Chemical shifts should be listed consistently in a single article, starting either from downfield to upfield or vice-versa. Assign peak identities under the following circumstances: non-decoupled or equivalent spectra have been collected (<sup>13</sup>C, <sup>31</sup>P, etc.); 2-D experiments have been performed; or unambiguous assignment is possible without additional experiments, such as in the case of an organometallic metal-hydride <sup>1</sup>H signal, PF<sub>6</sub> vs MPPH<sub>3</sub> <sup>31</sup>P signal, etc. Give <sup>13</sup>C chemical shifts to one digit after the decimal point, unless an additional digit will help distinguish overlapping peaks. Include peak multiplicities for <sup>1</sup>H-coupled <sup>13</sup>C NMR spectra or for signals in <sup>1</sup>H-decoupled spectra that are coupled to other magnetically active nuclei. A <sup>13</sup>C NMR signal will be considered a singlet if the multiplicity is not assigned. Only rarely is a true multiplet observed in



a  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum. However, a certain region may contain a group of unresolved peaks or signals. Mention of unobserved resonances is encouraged.

See '[Supporting Information](#)' below for instructions about submission of spectra.

**Structural and Chemical Shift Data for Proteins and Nucleic Acids.** Any set of atomic coordinates referred to in the manuscript, including atomic coordinates and structure factors for proteins determined by X-ray crystallography and coordinates determined by NMR, should be deposited with the Protein Data Bank, Research Collaboratory for Structural Bioinformatics at Rutgers University whenever appropriate. (Theoretical model depositions are no longer accepted for inclusion in the PDB archive.) If the coordinate files are not deposited in the PDB, or if the PDB files are on hold until publication, then the coordinate files must be included in the Supporting Information submitted concurrently with the manuscript. Requirements are similar for structures of nucleic acids, which should be deposited with the Nucleic Acid Database. A manuscript that does not provide coordinates at the time of submission will not be sent out for review. It is the responsibility of the author to obtain a file name (PDB ID or NDB ID) for the molecule; the file name must appear in the published manuscript. If a file name has not yet been obtained upon acceptance of a paper, it must be added in proof. Atomic coordinates and structure factors for all structures mentioned must be available immediately upon publication of the paper, either directly in the Supporting Information or as a data bank deposition. Similar requirements also apply to any chemical shifts referred to in the paper, whether they are only for assignment of resonances or used for any form of structure calculation. Those chemical shifts must be available to the reviewer at time of submission, either as an available entry in the Biological Magnetic Resonance Data Bank or included directly as Supporting Information.

**Single Crystal Diffraction Data.** Manuscripts reporting the determination of one or more structures by X-ray diffraction must adhere to the following requirements:

*Abstract.* The abstract may summarize geometric features of unusual interest but should not contain unit cell parameters.

*Main Body of Manuscript.* Tables of essential interatomic distances and angles are *not required* but may be submitted (metric information for standard structural components should not be included).

For structures with anisotropically refined atoms, a figure displaying the thermal ellipsoids should ordinarily be presented; a spherical-atom representation may be substituted if necessary for clarity. If a spherical atom view is chosen for the manuscript, a thermal ellipsoid figure should be included in the Supporting Information. In cases where intermolecular interactions are relevant to the discussion, a view of the unit cell may be included.

An Article should list for each structure the formula, formula weight, crystal system, space group, color of crystal, unit cell parameters, temperature of data collection, and values of  $Z$ ,  $R$ , and GOF; a brief description of data collection and solution and refinement of the structure should be placed in the Experimental Section. Tables of atom coordinates and thermal parameters will not be printed.

*Supporting Information.* Complete detailed data for each structure must be submitted in the electronic Crystallographic Information File (CIF) format. Deposition of CIF files in the

Cambridge Crystallographic Data Centre (CCDC) does not eliminate the *JACS* requirement to submit the CIF file(s) as Supporting Information.

Authors are requested to combine multiple CIFs for a given manuscript into a single file. The individual structures in the combined file are to be separated from each other by the sequence #===END at the beginning of a new line. *JACS* requires authors to run the CheckCIF program for each crystallographic structure and to correct any syntax errors in the CIF file prior to submission. Authors should consult the *JACS* [Information for Authors](#) for CIF Submission Instructions **during manuscript preparation**.

Structure factors (except for proteins and nucleic acids) should not be submitted as Supporting Information. However, one printed table of structure factors should be retained in case it is requested by the Editor for review purposes only.

**Powder Diffraction Data.** The presentation of X-ray powder diffraction data for new materials or for materials previously uncharacterized by this technique is encouraged. Data from X-ray powder measurements should be accompanied by details of the experimental technique: source of X-rays, the radiation, its wavelength, filters or monochromators, camera diameter, the type of X-ray recording, and the technique for measuring intensities. In cases of unindexed listing of the data, the  $d$  spacings of all observed lines should be listed in sequence, together with their relative intensities. In cases where filtered radiation is used, every effort should be made to identify residual  $\beta$  lines. Where resolution into  $\alpha_1$ - $\alpha_2$  doublets occurs, the identification of the  $d$  spacing for each line as  $d\alpha_1$ ,  $d\alpha_2$  gives a measure of the quality of the diffraction pattern. When an indexing of the data is offered, the observed and calculated  $1/d^2$  values should be listed along with the observed relative intensities (it is superfluous to give  $d$  spacings in this instance). All calculated  $1/d^2$  values should be listed (exclusive of systematic absences), to the limit of the data quoted. If possible, the crystal system should be specified. Possible space groups may also be listed if the data warrant it. Relevant information about the specimen used should be included.

**Magnetic Measurements.** Fits of magnetic data [ $\chi(T)$ ,  $\chi^{-1}(T)$ ,  $\chi T(T)$ ,  $\mu(T)$ ,  $M(H)$ , etc.] to an analytical expression must include both the Hamiltonian from which the analytical expression is derived and the final analytical expression and fitting parameters. When the value of an exchange coupling constant,  $J$ , is given in the abstract, the form of the Hamiltonian must also be included. The expressions may be included in the manuscript or, if long and complex, as Supporting Information; if the latter method is used, it should be noted in the Supporting Information paragraph at the end of the manuscript. In addition, how the sample was measured (in a gelatin capsule, Teflon capsule, etc.) and the diamagnetic correction for the sample holder, as well as the diamagnetic correction for the material, must be provided and the manner in which it was calculated (Pascal's constants) or measured must be stated.

**Computations.** When computational results are an essential part of a manuscript, sufficient detail must be given, either within the paper or in the Supporting Information, to enable readers to reproduce the calculations. This includes data such as force field parameters and equations defining the model (or references to where such material is available in the open literature). If the software used for calculations is generally available, it must be properly cited in the References and Footnotes. References to the methods upon which the software is based must also be provided. Results obtained from methods or parameters that are not adequately described in the manuscript or in the literature are not acceptable for publication. Authors who report the results of electronic structure calculations are requested to provide as Supporting Information the

geometries (either as Cartesian coordinates or Z matrices) of all the stationary points whose relative energies are given in the manuscript. The absolute energies in hartrees that are computed at these geometries should not be given in the manuscript but should be included in the Supporting Information. Where applicable, the number of imaginary frequencies should be reported to identify stable structures and transition states.

## Supporting Information

**General Considerations.** Material that is not needed for reading the paper but which should be available to document experiments or calculations for future researchers should be put into the Supporting Information. This material may include tables, illustrations, derivations, experimental procedures, analytical and spectral characterization data, spectra, modeling coordinates and programs, and crystallographic information files. Videos/movies may be included as Supporting Information, but authors should consider whether they would be better featured as Web Enhanced Objects (WEOs), particularly if they are directly related to specific figures or discussion in the text. The Supporting Information may also include additional material or discussion that is primarily of interest to specialized readers.

Appendices must appear in the Supporting Information and not in the manuscript file. Authors are encouraged to make use of Supporting Information in the interest of shorter Articles, not only to save space but also to create more focused presentations.

Material deposited as Supporting Information is considered to be part of the publication and should not be submitted for republication as part of a future paper.

The Supporting Information will be made available free of charge on the Web.

Text and tabular material should be double-spaced; graphics should be saved at a resolution that allows clear viewing on the Web. The templates available for preparing Articles may also be used for producing Supporting Information. The page size should be (U.S. Letter) 8.5 in. × 11 in. (22 cm × 28 cm), and the readable material should be aligned parallel with the 8.5 in. (22 cm) dimension wherever possible.

All pages of the PDF file should be numbered consecutively starting with page S1. Pages of CIF and other file types need not be numbered.

**NMR Spectra.** Submission of spectra (.doc, .docx, .txt, .pdf, .tif) is strongly recommended for all new and/or key compounds, following these guidelines:

- A caption should be included on the spectrum, noting the nucleus being measured, the solvent (formula preferred, e.g. C<sub>6</sub>D<sub>6</sub> over benzene-*d*<sub>6</sub>) and the field strength.
- A representation of the compound should be included on the spectrum—please use ChemDraw or a related program. The compound identifier used in the manuscript should be included.
- The largest peak in the <sup>1</sup>H NMR spectrum should normally arise from the compound, not the solvent.
- All peaks in the <sup>1</sup>H NMR spectrum should be integrated. Chemical shift values should be included.

- The solvent peak should be clearly labeled on the spectrum.
- All peaks should be visible on the spectrum. Insets are encouraged to show expanded regions. At minimum, the spectral window should be -1 ppm to 9 ppm for  $^1\text{H}$  NMR and -10 ppm to 180 ppm for  $^{13}\text{C}$  NMR.
- Font should be clear and large enough to read (minimum of 10 point). Horizontal orientation is preferred for spectra.

Submission of primary NMR data files (FID files, acquisition data, processing parameters) is encouraged for all new and/or key compounds. When submitting these files, please consider the following guidelines:

- One folder should be created for each compound. The folder should be named clearly, using the compound name (if available) and compound identifier, as referenced in the Experimental Section or Supporting Information. Include the FID files, acquisition data, and processing parameters for each experiment.
- Name each spectrum according to the type of nucleus measured.  $^1\text{H}$ ,  $^{13}\text{C}$ , DEPT, COSY, etc. NMR files should be compressed into zip files—please use multiple zip files if necessary. Files must be submitted in their native format. In a text document, include the name of the manufacturer of the spectrometer used to collect the data, the acquisition software and processing programs used to analyze the data, and the field strength used to measure each nucleus (i.e. 300 MHz  $^1\text{H}$  or 50 MHz  $^{13}\text{C}$ ). Include a structure file that shows the structure and compound identifier for each provided dataset. MolFile is the recommended format and is strongly preferred.

**Nuclear Magnetic Resonance Pulse Sequences.** For manuscripts that present new NMR pulse sequences, authors are requested to supply as “Supporting Information for Publication” a file that includes the original working pulse sequence information required to record data. This will typically include the pulse sequence code, parameter set, and other associated files, such as tables of gradient or pulse shapes.

**Submission.** Supporting Information must be submitted at the same time as the manuscript and uploaded separately to the ACS Paragon Plus Environment. A [list of acceptable file types](#) is available on the Web. All Supporting Information files of the same type should be prepared as a single file (rather than submitting a series of files containing individual images or structures). For example, all Supporting Information available as PDF files should be contained in one PDF file. Whenever possible, all text and graphics in the Supporting Information should be consolidated into a single word-processing file.

**DO NOT UPLOAD CONTENT THAT IS TO BE PUBLISHED IN THE ARTICLE INTO THE SUPPORTING INFORMATION FILE(S).**

**Access to Supporting Information.** Supporting Information from 1993 to the present is available free of charge from the [JACS home page](#). SI prior to 1993 is available, for a fee, from Publications Support Services. Tel: (202) 872-4376. Fax: (202) 872-6325. E-mail: [pss@acs.org](mailto:pss@acs.org).