ACS Publications

ACS Catalysis

Information for Authors

(August 2011)

Contents (click on the topic)

Scope and Editorial Policy

I. General Considerations

ACS Catalysis is an interdisciplinary journal publishing original research on and at the interfaces of heterogeneous catalysis, homogeneous catalysis, and biocatalysis. Application coverage of *ACS Catalysis* will include life sciences, drug discovery & development, household products, polymer discovery & production, environmental protection, chemical production, energy & fuels, and other areas. The journal is devoted to reports of new and original experimental and theoretical research on molecules, macromolecules or materials that are catalytic in nature (exhibiting catalytic turnover) and they should be characterized to the extent possible by turnover frequencies and fundamental kinetic parameters. Manuscripts that are essentially reporting data or applications of data are, in general, not suitable for publication in *ACS Catalysis.* All manuscripts are subject to evaluation by the Editor and/or Associate Editors prior to peer review, and manuscripts sufficiently lacking in novelty or new insights may be, on occasion, rejected without external peer review. In such instances, these decisions will be made expediently, so as to not delay publication elsewhere. Before publication, all manuscripts, including invited contributions, are subject to critical, anonymous peer review. Reviewers are advisory to the Editor. It is understood that the final decision relating to a manuscript's suitability rests solely with the Editor.

Notice: Accepted manuscripts will be published on the "Articles ASAP" page on the Journal Web site as soon as page proofs are corrected and all author concerns are resolved. Publication on the Web usually occurs within 4 working days of receipt of page proof corrections, and this can be anywhere from 2 to 11 weeks in advance of the cover date of the issue. 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.

Corresponding authors will receive 50 free electronic reprints via an Electronic Reprint URL. There are no page charges associated with *ACS Catalysis.*

II. Types of Manuscripts

ACS Catalysis publishes five types of papers: Letters, Articles, Perspectives, Reviews, and Viewpoints. Correspondence and Additions and Corrections are also published.

A. Letters are short articles that report results whose immediate availability to the science and engineering community is deemed important. Letters are restricted to 2000 words or the equivalent (8 double-spaced typewritten pages of text and 4–5 figures). A brief abstract of less than 100 words should be included. Letters often will be complete publications, but follow-up publication may occasionally be justified when the research is continued and a more complete account of the work is deemed necessary. Special efforts will be made to expedite the reviewing and the publication of Letters. The time for proofreading the galley proofs is relatively short. For this reason, authors of Letters should ensure that manuscripts are in final, error-free form when submitted.

B. Articles should cover their subjects with thoroughness, clarity, and completeness but should be as concise as possible. Abstracts to Articles are limited to 300 words and should summarize the significant results and conclusions.

C. Perspectives are short reviews of recent developments in an established or developing topical area. Authors may be invited by the Editor to submit Perspectives. Unsolicited Perspectives will be considered, as well; however, 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 review topic. One-page proposals should be sent to the Editor-in-Chief, Christopher Jones (EIC@catalysis.acs.org) for consideration.

D. Reviews are comprehensive, critical examinations of a selected topic, typically over a defined time period. Unsolved problems and emerging areas should be highlighted. A Review should consist of a maximum of 40 pages (approximately 65000 characters) of main text, footnotes, literature citations, tables, and legends. Most Reviews are expected to be substantially shorter in length, but the length will be dictated by the subject matter to some degree. Authors may be invited by the Editor to submit Reviews. Unsolicited Reviews will be considered as well; however, authors interested in submitting a Review are strongly encouraged to contact the Editor prior to manuscript preparation and submission, to seek conditional approval of the proposed review topic. One-page proposals should be sent to the Editor-in-Chief Christopher Jones (EIC@catalysis.acs.org) for consideration.

E. Viewpoints appear mostly as a result of an invitation from the Editor and will be so designated. These articles normally will be in highly active research areas, and they are not intended to be reviews of the literature. The author will be asked to provide a clear, concise, and critical status report of the field as an introduction, and the author's own contribution to the field should constitute the main body of the article. Authors in highly active research fields of broad interest in catalysis are encouraged to propose Viewpoints.

F. Correspondence/Rebuttal. Correspondence is a technical contribution providing, with supporting material, a respectful but alternative point of view to one that has appeared in *ACS Catalysis.* The author of the original publication may be invited to write a Rebuttal. The Correspondence and Rebuttal will appear in the same issue of the journal.

Additions and Corrections should be submitted by the corresponding author if errors of consequence are detected in the published paper. An addition or correction may be submitted via the ACS Paragon Plus Environment (select "Additions and Corrections" as the manuscript type). All Additions and Corrections are subject to approval by the Editor, and minor corrections and additions will not be published. Additions and Corrections may not be submitted by anyone other than the corresponding author of the paper requiring correction. The corresponding author should obtain approval from all coauthors prior to submitting an addition or correction. Readers who detect errors of consequence in the work of others should contact the corresponding author of that work.

III. Functions of Reviewers

The Editor requests the scientific advice of reviewers who are active in the area of research and development covered by the manuscript. The reviewers act only in an advisory capacity, and the final decision concerning a manuscript is the responsibility of the Editor. The reviewers are asked to comment not only on the scientific content but also on the manuscript's suitability for *ACS Catalysis.* With respect to Letters*,* the reviewers are asked to comment specifically on the urgency of publication. **Authors must suggest, when submitting a manuscript, names and e-mail addresses of at least four scientists who could give a competent and objective evaluation of the work.** All reviews are anonymous, and the reviewing process is most effective if reviewers do not reveal their identities to the authors. An exception arises in connection with a manuscript submitted for publication in the form of a comment on the work of another author. Under such circumstances, the first author will, in general, be allowed to review the communication and to write a rebuttal. The rebuttal and the original communication may be published together in the same issue of the journal.

IV. Revised Manuscripts

A manuscript sent back to an author for revision should be returned to the Editor as soon as possible. If a revision is not received within **21 days**, it will be considered withdrawn. Revised manuscripts are sometimes sent back to the original reviewers, who are asked to comment on the revisions. If only minor revisions are involved, the Editor will examine the revised manuscript in light of the recommendations of the reviewers without seeking further opinions. A letter from the author must accompany the revised manuscript and provide a detailed account of how the author has responded to the reviewer's comments. The dates of receipt of the original and revised manuscripts will both appear in publication.

Preparation of Manuscripts

Submission of Manuscripts

Manuscripts must be submitted via the ACS Paragon Plus Environment (http://paragonplus.acs.org/login). Complete instructions and an overview of the electronic online (Web) submission process are available through the secure ACS Paragon Plus Web site. Authors will view the PDF version of their manuscripts prior to formal submission to the Editor. In response to the request for revision from the Editor, authors must also submit all revisions and final, accepted manuscripts via the ACS Paragon Plus Environment. The supported platforms and word processing packages are listed in the *ACS Catalysis* Web home page via http://pubs.acs.org/accacs. To use Web submission, authors must be able to provide

electronic versions of text and graphics. Any Supporting Information should also be submitted electronically.

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 manuscript.

Authors are asked to embed graphics in the text. A mechanism is also provided for submitting an electronic cover letter to the Editor. Authors will be sent a message by e-mail acknowledging receipt of the manuscript. **Manuscripts submitted as e-mail attachments will not be accepted.**

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..

Table of Contents Graphic

A graphic must be included with each manuscript for the Table of Contents (TOC), which will also be used as the Abstract graphic. This graphic should capture the reader's attention and, in conjunction with the manuscript title, should give the reader a quick visual impression of the essence of the paper without providing specific results. The TOC graphic should be in the form of a structure, graph, drawing, SEM/TEM photograph, or reaction scheme. The author must submit a graphic in the actual size to be used for the TOC that will fit in an area 1.5 in. high and 3.33 in. wide (3.81 cm × 8.46 cm). Larger images will be reduced to fit within those dimensions. Type size of labels, formulas, or numbers within the graphic must be legible. Tables or spectra are not acceptable. Provide the TOC graphic upon submission of the paper as the last page of the manuscript.

Cover Letter

A letter **must** accompany the manuscript, and it **must** contain the following elements. Please provide these elements in the order listed.

- A paragraph explaining why your manuscript is appropriate for *ACS Catalysis.* This paragraph should clearly indicate what application is described in the work.
- If the manuscript was previously rejected by *ACS Catalysis,* provide the manuscript number of the rejected manuscript and a detailed response to each reviewer's comments.
- If the manuscript was previously rejected by any other ACS journal, provide the name of the journal, the manuscript number, an explanation of the basis for the rejection, and a statement granting *ACS Catalysis* permission to obtain the Editor's decision letter and review for the rejected manuscript. Also indicate if the newly submitted manuscript has

been revised based on the previous reviews. If so, provide a detailed response to each reviewer's comments.

- A statement confirming the manuscript, or its contents in some other form, has not been published previously by any of the authors and/or is not under consideration for publication in another journal at the time of submission.
- A description of any supporting information and/or Review-Only Material.
- The names and e-mail addresses of four possible reviewers.

Submission Details

The following information is required for manuscript submission in the ACS Paragon Plus Environment:

- **Type of Manuscript** (Letter, Article, Perspective, Review, Viewpoint, Correspondence, or Addition and Correction)
- **Manuscript title**
- **Abstract**
- **Verification of Authorship or Submitting Agent**
- **Name and contact information (including e-mail address) of the Corresponding Author**
- **Name(s) and contact information (including e-mail address) of all other authors**

Precautions for handling dangerous material or for performing hazardous procedures should be explicitly stated.

Submitting Artwork for the Journal Cover

ACS Catalysis features a different image on the cover of each issue. The image is usually related to work that is published in that particular issue. Authors are encouraged to submit images to be considered for use on future covers at the time of the initial submission of their manuscript.

Images to be considered for the cover should be submitted as TIF, EPS, or high-resolution PDF files with a resolution of at least 300 dpi for pixel-based images. The image size is 8.5 in × 8.8 in., 21.6 cm × 22.4 cm, or 2530 pixels × 2640 pixels. More information may be found in the Digital Image Guidelines for Journal Cover Graphics in the ACS Paragon Plus Environment. Please include a separate Journal Publishing Agreement (for unpublished images) or written permission to reproduce in all media (for previously published images) for each image submitted, the name of the person who created the image, and a brief description of the image. Copyright and Permission Request forms are available on the Publications Division Web site, at http://pubs.acs.org/copyright.

Just Accepted Manuscripts

Just Accepted manuscripts are peer-reviewed, accepted manuscripts that are posted on the ACS Publications website prior to technical editing, formatting for publication, and author proofing—usually within 30 minutes to 24 hours of acceptance by the editorial office. During the manuscript submission process, Authors can choose to have their manuscript posted online as a *Just Accepted* manuscript. To ensure rapid delivery of the accepted manuscript to the Web, Authors must adhere carefully to all requirements in the journal's

Information for Authors. For further information, please refer to the *Just Accepted* FAQ, at http://services.acs.org/pubshelp/passthru.cgi?action=kb&item=244. Note that publishing a manuscript as *Just Accepted* is not a means by which to comply with the NIH Public Access Mandate.

Related Work by Author

All related work under consideration for publication in any medium must be cited in the manuscript and the Editor 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 *ACS Catalysis* or another journal, a copy of each related paper should be uploaded as "Supporting Information for Review Only" at the time of submission for use by the reviewers and the Editors. If a cited reference has already appeared on the Web, indicate that it is published electronically ("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.

Elements of Manuscripts

Authors should consult a recent issue of *ACS Catalysis* and *The ACS Style Guide*, 3rd ed. (2006) Oxford University Press, Order Department, 201 Evans Road, Cary, NC 27513, for formal guidance. Any author who is not fluent in idiomatic English is urged to obtain assistance with manuscript preparation from a fluent colleague because manuscripts with grammar deficiencies are sometimes handicapped during the scientific review process.

Title

Titles should clearly and concisely reflect the emphasis and content of the paper. Titles are of great importance for current awareness and information retrieval and should be carefully constructed for these purposes. Titles of manuscripts may not contain the word "First" or "Novel" nor any part number or series number.

Author List

Bylines should include all those who have made substantial contributions to the work. To facilitate indexing and retrieval and for unique identification of an author, use first names, initials, and surnames (e.g., John R. Smith) or first initials, second names, and last names (e.g., J. Robert Smith). At least one author must be designated with an asterisk to indicate the person to whom readers may send correspondence. Deceased persons who meet the criterion for inclusion as co-authors should be so included, with a footnote indicating the date of death.

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, the current address should be given in a footnote. The e-mail address(es) of the corresponding author or authors must also be provided as a separate line below the institution addresses.

Abstract

All Articles, Letters, Perspectives, and Reviews must be accompanied by an abstract, including an Abstract graphic, which should state briefly the purpose of the research (if this is not contained in the title), the principal results, and major conclusions.

Keywords

All Articles, Letters, Perspectives, and Reviews must be accompanied by 5–8 keywords. These keywords will appear in the PDF version of the article and will also be used as a search term in the HTML version of the article.

Text

All sections of the paper must be presented in a clear and concise manner. Authors should include an introductory statement outlining the scientific motivation for the research. The statement should clearly specify the questions for which the answers are sought as well as the connection of the present work with previous and current work in the field. In both Letters and Articles, the introduction should be a separate section of the paper. In the discussion section, the author should discuss the significance of his/her observations, measurements, or computations. The author should also point out how they contribute to the scientific objectives indicated in the introduction. Tabulation of experimental results is encouraged whenever it leads to a more effective presentation or economical use of space. Authors are encouraged to make extensive use of the Supporting Information format, because this material is now widely available on the Web at http://pubs.acs.org.

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.

Figures. All figures must be mentioned in the text in consecutive order and must be numbered with Arabic numerals. A caption giving the figure number and a brief description, preferably only one or two sentences, must be included. 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. Ensure that any symbols and abbreviations used in the text agree with those in the artwork.

Schemes. Sequences of reactions are called schemes and should be numbered consecutively with Arabic numerals. Schemes may have brief titles describing their contents and footnotes, if needed, for further detail. Schemes should be numbered with Arabic numerals in consecutive order.

Charts. Groups of structures that do not show reactions are called charts and should be numbered consecutively with Arabic numerals. Charts may have brief titles describing their contents and footnotes, if needed, for further detail.

Tables. 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.

Tables should be numbered consecutively with Arabic numerals and placed in the text near the point of first mention. 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. 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.

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 which refers to the numbered reference in the text should be placed in the table.

In setting up tables, authors should keep in mind the type area of the *ACS Catalysis* page (17.8 cm × 23.5 cm) and the column width (8.5 cm) and should make tables conform to the limitations of these dimensions.

Compound Characterization, Experimental and Computational Data

Authors are required to provide sufficient information (as described in more detail below) to establish the identity of a new compound, its purity, and its yield. Sufficient experimental details must also be included to allow another researcher to reproduce the synthesis. Characterization data and experimental details must be included in either the paper or the Supporting Information.

Guidelines for Characterization of Organometallic and Inorganic Compounds.

(a) Routine Compounds

Compounds in this category are those that have either literature precedents or are obtained by a logical synthesis in close to quantitative yield. Sufficient data must be provided to identify and verify the structure of such compounds.

(b) Novel or Unexpected Compounds

Compounds in this category are those that either (i) exhibit an unprecedented type of structure, or (ii) are obtained by unexpected reaction. Such compounds require more detailed characterization to ensure their validity. In select instances, a variety of definitive spectroscopic techniques may provide sufficient characterization (for example, if many of the nuclei are NMR active), but in the majority of cases evidence for elemental constitution must be provided by either elemental analysis or mass spectrometry. While an X-ray diffraction structure is not considered definitive proof of elemental composition, it is acceptable evidence for composition providing that the results of other physical methods concerning the characterization are conclusive.

(c) Solid State Materials

Compounds in this category are those that have no existence in solution. Solid state materials, such as heterogeneous catalysts, must be characterized in such a way as to sufficiently describe their structure and composition. Atomic ratios and elemental compositions must be provided for solid state materials. X-ray diffraction data should be provided for crystalline materials.

(d) Compounds That Have Not Been Isolated

Compounds that have not been isolated in pure form (e.g. reaction intermediates or intractable mixtures, or unstable species) may be published. However, in these circumstances, an explicit statement must be given indicating that the compounds have not been isolated. Only in exceptional circumstances will a paper be published in which none of the new compounds reported has been isolated and fully characterized.

(e) Purity and Yield

The yield and purity of all molecular species must be reported, including the methods used to determine them. The yield of a compound obtained in an NMR tube reaction should be determined using an internal standard.

Guidelines for Characterization of Organic Compounds

(a) Sample Quality

For new substances, evidence of the homogeneity of the purified sample should be included. Elemental analysis is sufficient. If no analysis was performed, then other evidence (for example, ^{1}H NMR, ^{13}C NMR, HPLC, GLPC, gel electrophoresis, etc.) should be included as figures in the Supporting Information.

(b) Molecular Weight

Evidence of molecular weight should be provided, especially if elemental analysis is not performed. Low resolution MS data under conditions that minimize fragmentation are acceptable. If there is a specific need to distinguish alternative formulas with the same molecular mass (within one amu), then HRMS data are necessary.

(c) Miscellaneous

Numerical listings of characteristic spectroscopic data should be included to support assigned structures, changes in functionality, unusual chromophores, etc. Methods of purification used to prepare samples for characterization should be described. For crystalline samples, information about the method of crystallization should be included (solvents; mp; etc.). For non-racemic, chiral substances, data to allow correlation of absolute configuration should be given, preferably including $[\alpha]_D$ values. If correlation data are provided based on HPLC or GLPC methods, then retention times for both enantiomers must be provided, together with solvent and flow rate information, and identification of the chiral support.

(d) Intermediates on Solid Phase; Combinatorial Chemistry

Validation of methods and characterization of new substances in a statistically significant sampling should be provided. Resin-bound intermediates need not be characterized if acceptable end product quality (as defined in a–c above) is demonstrated.

Kinetic and Equilibrium Data

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.strenda.org/documents.html) for an example of detailed guidelines.

Structural Data for Proteins and Nucleic Acids

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. Theoretical model depositions are no longer accepted for inclusion in the PDB archive. Structures of nucleic acids should be deposited with the Nucleic Acid Database. 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. A manuscript will be sent out for review without the file name only after receipt from the submitting author of a written statement that the coordinates will be deposited. 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 must be released immediately upon publication of the paper.

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 Supporting Information. Tables of atom coordinates and thermal parameters will not be printed.

CIF Submission Instructions

If single crystal X-ray structures are reported, authors are required to submit X-ray crystallographic data to be published as Supporting Information. The information required for each structure should be submitted in the electronic Crystallographic Information File (CIF) format. Such files should be submitted electronically as described below.

CIFs must be uploaded at the same time the manuscript is submitted via the Web, with the file designation Supporting Information for Publication. The CIF for each structure should be uploaded as a separate Supporting Information file. CIFs should be saved in the text-only (plain ASCII) format, with a .cif extension before being submitted. No information other than the CIF itself should be included inside the file. CIFs may NOT be furnished as Microsoft Word, Corel WordPerfect, or PDF files.

Before submission, CIFs must be checked using the CheckCIF utility on the Web at http://checkcif.iucr.org/. A copy of the output should be retained in case it is requested by an Editor. Authors with appropriate software may alternatively use IUCRVAL or the CHECK validation tool in PLATON.

If CIFs are not available, the required data should be furnished in neatly formatted tables with informative titles that identify the name or the structure number of the compound.

Powder Diffraction Data

No special instructions apply to the use of X-ray powder diffraction in a routine manner to characterize heterogeneous catalysts. However, for new crystalline materials or for crystalline materials previously uncharacterized by this technique, specific guidelines are given here. In such cases, 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 β lines. Where resolution into α1–α2 doublets occurs, the identification of the d spacing for each line as dα1, dα2 gives a measure of the quality of the diffraction pattern. When an indexing of the data is offered, the observed and calculated 1/d2 values should be listed along with the observed relative intensities (it is superfluous to give d spacings in this instance). All calculated 1/d2 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.

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. 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.

Dedications

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

Acknowledgment

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

Supporting Information Statement

A brief statement in non-sentence format, which lists the contents of material placed in Supporting Information, should be included at the end of the manuscript (after the Acknowledgment and before the References and Footnotes). For instructions on what material should be provided as Supporting Information and on preparing it for publication, see the "Supporting Information" section below.

References and Footnotes

References and explanatory notes should be grouped at the end of the manuscript and typed double spaced. They should be numbered consecutively in the order in which they are first mentioned in the text. Each article cited in a manuscript should receive its own numeral. Compound references are not permitted. Papers should not depend for their usefulness on unpublished material, and excessive reference to material in press is discouraged.

Reference Format. The following format for journals (1) and books (2) must be used:

(1) Balsara, N. P.; Fetters, L. J.; Hadjichristidis, N.; Lohse, D. J.; Han, C. C.; Graessley, W. W.; Krishnamoorti, R. *Macromolecules* **1999**, 32, 6137-6147.

(2) Wignall, G. D. In *Encyclopedia of Polymer Science and Engineering*, 2nd ed.; Mark, H. F., Bikales, N. M., Overberger, C. C., Menges, G., Eds.; Wiley-Interscience: New York, 1999; Vol. 10, p 112.

Consult *The ACS Style Guide*, 3rd ed. (American Chemical Society: Washington, DC, 2006), available from Oxford University Press, for specific examples of styles and general recommendations. Authors are responsible for the accuracy of the references. Because subscribers to the Web edition are now able to click on the "CAS" tag following each reference to retrieve the corresponding abstract at Chemical Abstracts Service, reference accuracy is critical.

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. For references only available online at the time of submission, please provide the DOI number. Actual citation should be included before publication, if possible.

Nomenclature

Nomenclature should conform to current American usage. Insofar as possible, authors should use systematic names similar to those used by Chemical Abstracts Service and the International Union of Pure and Applied Chemistry. Chemical Abstracts (CA) nomenclature rules are described in Appendix IV of the Chemical Abstracts Index Guide. For CA nomenclature advice, consult the Manager of Nomenclature Services, Chemical Abstracts Service, P.O. Box 3012, Columbus, OH 43210-0012. A name generation service is available for a fee through CAS Client Services, 2540 Olentangy River Road, P.O. Box 3343, Columbus, OH 43210-0334; Telephone: (614) 447-3870; Telefax: (614) 447-3747; or E-mail: answers@cas.org.

Supporting Information

Authors are strongly encouraged to use Supporting Information to submit extensive tables, graphs, spectra, mathematical derivations, expanded discussion of peripheral points, or other material that, although essential to the specialized reader who needs all the data or all the detail, does not help and often hinders the effective presentation of the work being reported. The Supporting Information will be included in the Web edition of the journal and is available free of charge to the public. Authors are encouraged to make use of this resource, in the interest of shorter articles (which mean more rapid publication) and clearer, more readable presentation.

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. The Supporting Information should be preceded by a cover page that provides the title, authors, and corresponding author's contact information. Crystallographic information files must be furnished in CIF format in the Supporting Information, even if they have previously been submitted to the Cambridge Crystallographic Data Centre. All pages of the Supporting Information PDF should be numbered consecutively starting with page S1. Pages of CIF and .txt documents should not be numbered.

Do not upload figures and tables that are to be published in the article into the supporting information file.

A paragraph should appear at the end of the paper indicating the nature of the material and the means by which the interested reader may obtain copies directly. Use the following format:

> *Supporting Information Available*: Description of the material. This material is available free of charge via the Internet at http://pubs.acs.org.

Artwork

General Considerations. Graphics provided in color will be published in color (see the Color section below for details). Insert your illustrations into the manuscript following the Web instructions for manuscript preparation. See http://pubs.acs.org/page/accacs/submission/index.html for additional guidance. Illustrations must fit a one- or two-column format on the journal page: **For efficient use of journal space, single column illustrations are preferred. For best results, submit illustrations in the actual size at which they should appear in the journal.** Original illustrations that do not need to be reduced to fit a single or double column will yield the best quality. Lettering should be no smaller than

4.5 points. (Helvetica or Arial type works well for lettering.) Lines should be no thinner than 0.5 point. Lettering and lines should be of uniform density. If you must submit artwork that must be reduced, use larger lettering and thicker lines so that, when reduced, the artwork meets the above-mentioned parameters. Avoid using complex textures and shading to achieve a three-dimensional effect. To show a pattern, choose a simple crosshatch design.

Color. Color reproduction will be provided at no cost to the author. Color illustrations should only be submitted if essential for clarity of communication. A surcharge of $100 per 100 reprints will be added to the standard cost of reprints.

Chemical Structures. Structures should be produced with the use of a drawing program such as ChemDraw. Structure drawing preferences (preset in the ACS Stylesheet in ChemDraw) are as follows:

(1) As drawing settings select:

chain angle	120º
bond spacing	18% of width
fixed length	14.4 pt (0.508 cm, 0.2 in.)
bold width	2.0 pt (0.071 cm, 0.0278 in.)
line width	0.6 pt (0.021 cm, 0.0084 in.)
margin width	1.6 pt (0.056 cm, 0.0222 in.)
hash spacing	2.5 pt (0.088 cm, 0.0347 in.)

(2) As text settings select:

font	Arial/Helvetica
size	10 pt

(3) Under the preferences choose:

units	points
tolerances	5 pixels

(4) Under page setup choose:

Paper	US Letter
Scale	100%

Authors using other drawing packages should, in as far as possible, modify their program's parameters so that they reflect the above guidelines.

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