Guidelines for Authors

Revised June 2007

MAJOR CHANGES FOR 2007

Manuscripts are submitted on the ACS Paragon Plus Web site.

The names of potential reviewers are entered on a Web form during the submission process, rather than included in the cover letter.

Notes must be prepared with the *JOC* Note template. They are limited in length to four pages.

Manuscripts that are ready to be reviewed when first submitted will receive priority for initial processing and assignment to an editor. A Priority Processing Requirements list summarizes the requirements a manuscript needs to meet to qualify for priority treatment. Manuscripts that are incomplete or misformatted will be given a new "Received" date after the requested data or revision is received.

Authors will have 45 days to submit the first revision requested following peer review.

For all new compounds, a copy of a ^{1}H NMR spectrum (and a ^{13}C spectrum, if available) should be included in the supporting information.

In reaction schemes, abbreviations for reagents, solvents, and reaction conditions should be placed above or alongside the reaction arrows rather than in footnotes.

When compounds are prepared under more than one set of experimental conditions, the labeling of the spectra in the supporting information should identify the conditions that produced the samples whose spectra are shown. NMR spectra should be labeled with the solvent and instrument frequency.

CONTENTS

1 Scope and Editorial Policy

1.1 Scope of the Journal

The Journal of Organic Chemistry (JOC) welcomes original contributions of fundamental research in all branches of the theory and practice of organic and bioorganic chemistry. In selecting manuscripts for publication, the editors place emphasis on the quality and originality of the work as well as the breadth of interest to the organic chemistry community.

1.2 Types of Papers Published

Manuscripts can be submitted as Articles or Notes:

Articles are comprehensive, critical accounts of the solution of significant problems.

Notes are concise accounts describing novel observations, new methods of wide applicability or interest, or focused studies of general interest. They must be prepared using the *JOC* Note template (see section 2.3.2) and are limited in length to four pages, including the table of contents graphic, abstract, experimental section, references and footnotes, tables, and manuscript graphics. The level of experimental rigor (including compound characterization) required for a Note is the same as that for an Article. Notes differ from Articles by having a narrower scope; they differ from letters or communications in having an experimental section. *Notes should not present preliminary results that the author intends to publish later in a more complete form.*

Perspectives—personal overviews of specialized research areas by acknowledged experts—are published only by invitation of the Editor-in-Chief.

Recent Reviews—bibliographic listings of review articles and specialized monographs—are prepared by the Journal's Recent Reviews Editor.

1.3 Manuscript Requirements

Manuscripts should be submitted on the ACS Paragon Plus Web site at http://paragonplus.acs.org. A manuscript submitted

to *The Journal of Organic Chemistry* must be based on original research by the authors and must not have been published elsewhere (including in conference proceedings, in an electronic conference, or on a Web site). **No other manuscript reporting the same results may be under simultaneous consideration by another journal**.

Articles based on work reported in a preliminary letter or communication are welcome *provided that they represent a substantial amplification and extension of the earlier work*, not merely the addition of experimental details or further examples. Such submissions may include new experimental procedures, additional data, significantly expanded discussion, and further conclusions. Results that were reported in the preliminary publication may be included when the author feels readers will benefit from having all the related data collected in a single paper. The letter or communication must be mentioned in the cover letter and cited in the manuscript, and a copy of the preliminary report and any associated supporting information must be furnished as supporting information for review only (see section 3.3.4) for the convenience of the reviewers and editors.

Manuscripts declined by other journals will be considered if their focus is appropriate for publication in *The Journal of Organic Chemistry*. Resubmission of manuscripts previously considered and declined by *The Journal of Organic Chemistry* is discouraged except when the editor has invited submission of a new manuscript reporting additional work. If the editor agrees to reconsider a rejected manuscript that has been rewritten to accommodate the reviewers' or editor's objections, the revision will be treated as a new submission, will be given a new "Received" date, and will be assigned to the same editor.

1.4 Cover Art

The cover of each issue of the Journal features author-submitted artwork, often a computer-generated graphic or a graphic−photograph montage, that is related to an Article or Perspective in that issue. The cover art appears in both the printed edition and on the Journal's Web site (http://pubs.acs.org/joc). The editors encourage authors to submit imaginative artwork that highlights an aspect of the work being reported. Submissions should measure 7 in. (18 cm) wide by 8 in. (20 cm) high, should have a minimum resolution of 300 dpi, and should be saved in TIFF or EPS format. Additional information about preparing cover art may be obtained from the Editor-in-Chief's office (e-mail: joc@chem.utah.edu). Artwork prepared for consideration as cover art should be e-mailed to the Editor-in-Chief after receipt of the related manuscript has been acknowledged.

1.5 Manuscript Evaluation

The editors have final authority regarding all decisions concerning submitted manuscripts. Although they generally seek the advice of scientific peers, they may decline without review manuscripts judged inappropriate for the Journal or in violation of the ACS Ethical Guidelines. Reviewers are asked to evaluate manuscripts on significance, scientific rigor, breadth of interest to the organic chemistry community, thoroughness of compound characterization, appropriateness of cited literature, and quality of writing. An editor will consider, but will not always follow, the recommendations of the reviewers.

If substantially the same manuscript has been previously submitted to another ACS journal, the author should disclose that information in the cover letter, attach copies of all the reviews to the cover letter, and explain what revisions have been made in response to the reviewer comments. The editor may request the names of the original reviewers and copies of the reviews from the editor of the other journal. The editor may accept the manuscript on the basis of the original reviews and the author's changes, seek additional reviews, or reject the manuscript without further review. An author who feels that the manuscript was inappropriately reviewed previously may explain in the cover letter why he or she feels the editor should request additional reviews from different reviewers.

An author may request that a certain person not be used as a reviewer. Such a request will be honored unless the editor feels that individual's opinion, in conjunction with the opinions of other reviewers, is vital for evaluating the manuscript. The names of the reviewers will not be revealed to authors.

If the reports of the reviewers are positive, the editor may request the author to furnish a revised manuscript appropriately addressing any reviewer and editor concerns. The editor may send the revised manuscript to the original reviewers or to new reviewers, or may reach a decision based on the original reviews and the author's response to them, without seeking further opinions.

1.6 Professional Ethics

The Journal expects editors, reviewers, and authors to adhere to the standards embodied in the American Chemical Society's *Ethical Guidelines to Publication of Chemical Research*. Those guidelines are available on the Paragon Plus Web site at http://pubs.acs.org/paragonplus/ethics/ and in the first printed Journal issue of the current year.

Authors are reminded of their obligation to obtain the consent of all their coauthors prior to submitting a manuscript for publication. If any change in authorship is necessary after a manuscript has been submitted, the corresponding author must e-mail or fax a copy of a signed letter to the Editor-in-Chief confirming that all of the original coauthors have been notified and have agreed to the change. If the change involves the removal of a coauthor's name, the corresponding author must, in addition, arrange for the coauthor involved to e-mail or fax a copy of a separate signed letter consenting to the change.

Authors who submit manuscripts to the Journal may be asked from time to time to review manuscripts submitted by other researchers. Authors who repeatedly decline requests to review for the Journal or renege on commitments to review may be asked to submit their future manuscripts to other journals.

1.7 Publication Dates

The Journal is published biweekly in printed and Web editions. The final versions of accepted Articles and Notes will usually be posted as *Articles ASAP* on the Journal's Web site within four working days of receipt of the author's page proof corrections. The date of this posting will appear in both the printed and Web editions of the Journal. Authors should take the *Articles ASAP* publication date into account when planning patent or other time-sensitive activities. Once a manuscript appears on the Web, it is considered published. After that point, any change must be submitted for publication as an addition or correction (see section 3.7).

2 Preparing the Manuscript and Supporting Information for Publication

2.1 Manuscript Organization

The sections of a manuscript for an *Article* are:

- Title
- Authors' names and institution or company names and addresses
- Corresponding author's e-mail address
- Table of Contents Graphic
- Abstract
- Introduction
- Results and Discussion [may be separate]
- Conclusions [optional]
- Experimental Section
- Acknowledgments [optional]
- Supporting Information Available statement [required if the manuscript is accompanied by any supporting information for publication]
- References and Footnotes.

These sections (except for the title and author information) should be clearly labeled with boldface headings. *The section headings "Introduction", "Results and Discussion", and "Conclusions" are not used in a Note.*

2.1.1 Title. The title should accurately, clearly, and concisely identify the subject and emphasis of the reported work. The wording of the title is important for current awareness alerting and for information retrieval. Words should be chosen carefully to reflect the content and to function as indexing terms. Abbreviations should be avoided.

2.1.2 Authors' Names and Institution Addresses. A consistent format should be used in listing the names of the authors, preferably given name, middle initial (if any), and surname. The name of the corresponding author(s) should be marked with an asterisk (*). The names and addresses of the institution(s) where the work was performed should be listed in the following paragraph. If not all the coauthors are at the same institution or department, the institutional affiliation of each author should be indicated by labeling the institution names, using the typographic symbols †, ‡, §, and ||, and placing those symbols as superscripts after the appropriate author names.

2.1.3 Corresponding Author's E-mail Address. The e-mail address of the corresponding author should be placed on a separate line below the institution addresses (if there are two corresponding authors, e-mail addresses for both should be listed). If a corresponding author is no longer at the institution where the work was performed, the first footnote, marked with an asterisk (*), should be that author's current address. All editorial correspondence concerning receipt, review, revision, and publication of a manuscript will be sent by e-mail to the coauthor designated as the corresponding author on the manuscript, even if the manuscript is submitted by a different individual.

2.1.4 Table of Contents Graphic. Preparation of the table of contents graphic is discussed in section 2.5.7.

2.1.5 Abstract. The abstract should briefly state the purpose of the research, the principal results, and the major conclusions. An 80- to 200-word abstract is usually adequate for an Article. The abstract for a Note is limited to a maximum of 80 words. A boldface "**Abstract**" heading should be provided for this section. Footnotes and undefined abbreviations should not be used in the abstract, but compounds discussed in the manuscript may be referred to by their structure numbers.

2.1.6 Introduction. The introduction should place the work in the appropriate context and clearly state the purpose and objectives of the research. An extensive review of prior work is not appropriate, and documentation of the relevant background literature should be selective rather than exhaustive, particularly if reviews can be cited. The introduction of an Article should require no more than two double-spaced manuscript pages. The opening paragraph of a Note (not labeled "Introduction") serves a similar function but should be much shorter.

2.1.7 Results and Discussion. The presentation of experimental details in the results and discussion section should be kept to a minimum. Reiteration of information that is made obvious in tables, figures, or reaction schemes should be avoided. Authors are encouraged to make extensive use of *supporting information for publication*, which is supplementary material that is submitted at the same time as the manuscript, is made available on the Journal's Web site, and is linked to the Article or Note in the Journal's Web edition. The use of supporting information is particularly appropriate for presenting additional discussion, graphs, spectra, and tables that are more likely to be of interest to specialists than to general readers. Section 2.6 ('Supporting Information for Publication') discusses the mechanics of preparing this material for submission.

2.1.8 Conclusions. If an optional conclusions section is used, its content should not substantially duplicate the abstract.

2.1.9 Experimental Section. This section, together with material furnished in the supporting information for publication, should describe experimental methods in sufficient detail to permit repetition of the work by others. Every manuscript reporting experimental work must include the experimental methods, key steps, or representative procedures in an experimental section; less critical experimental details should be included in the supporting information. *Manuscripts submitted without an experimental section* (other than those reporting solely theoretical work) *cannot be forwarded for review.* Section 2.2 ('Specialized Data') should be consulted for guidance on reporting synthetic experimental, compound characterization, spectroscopic, crystallographic, and computational data in the manuscript and supporting information.

Special attention should be called to hazardous compounds or operations, and appropriate precautions should be described.

General Experimental Methods. If a General Experimental Methods paragraph is optionally provided to document procedures (such as purification methods, solvent removal, and spectroscopic and chromatographic analyses) that are common to all or most of the individual procedures, it should be placed at the beginning of the supporting information for publication and should not be included in the experimental section. Alternatively, a reference to the General Experimental Methods paragraph in an earlier publication may be provided.

Sources of stationary phases for chromatography and supports for solid-phase synthesis may be identified. Sources of reactants, reagents, and solvents available from major laboratory chemical and biochemical supply firms should *not* be identified except in the case of starting compounds that are unusual or not widely available, or when the author has evidence that the use of material from a particular source is critical to the outcome of an experiment. Procedures requiring the use of an enzyme or reagent that is neither commercially available nor prepared by a published nonproprietary method, and the results of experiments in which it was used, may not be reported.

Manufacturers and model numbers of spectrometers, chromatographs, and other standard laboratory instruments should not be identified. Commercial and institutional providers of analytical services (or locations of instrument facilities) should not be named. *These policies apply to experimental details reported in both the experimental section and the supporting information.*

2.1.10 Acknowledgments. This section may be used to acknowledge discussions with other researchers, technical assistance, gifts of starting materials or reference samples, data from individual providers of spectroscopic, analytical, or crystallographic services who are not coauthors, and financial support. Authors whose cover art submissions are used may later add a recognition of the graphic artist.

2.1.11 Supporting Information Available Statement. If the manuscript is accompanied by any supporting information for publication, a brief description of the supporting information material is required in the manuscript. The appropriate format is "**Supporting Information Available:** [concise list of types of data being furnished.] This material is available free of charge via the Internet at http://pubs.acs.org." *The manuscript cannot be forwarded for review or publication if this statement is missing.*

2.1.12 References and Footnotes. *All the references and footnotes must be placed together in a single consecutively numbered list at the end of the manuscript text.* They should be numbered with Arabic numerals in the order of their first citation in the text, and the corresponding citation numbers should be inserted at the appropriate locations in the text as superscripted numerals without parentheses or brackets. During production of the printed edition of the Journal, the individual references and footnotes will be placed at the bottom of the columns in which they are first cited. In the HTML version in the Web edition, they will appear grouped together at the end of the text; many of the references will have links to the abstract and full text on publisher Web sites. Because of this electronic linking, and because the references are not checked in detail

by editors or reviewers, *it is crucial that authors verify their accuracy*.

Authors should be judicious in citing the literature; unnecessarily long lists of references should be avoided. If a number of publications are relevant to a statement in the text, not more than two or three of the most seminal or most recent ones should be cited; if appropriate, the author may add "and references cited therein" following a reference. Any articles, communications, letters, patents, theses, and conference abstracts in which portions of the reported work have been previously disclosed must be cited. Long footnotes should be avoided; additional data and peripheral discussion should be placed in the supporting information rather than in footnotes.

Authors should consult a recent issue of the Journal or *The ACS Style Guide* (3rd ed., 2006, Oxford University Press, ISBN 0-8412-3999-1; http://pubs.acs.org/books/styleguide) for guidance on the appropriate formats to use in citations of journal papers, books, and other publications. The names of all coauthors of a cited work should be listed ("et al." may be used in the text where the work is discussed). Journal title abbreviations should be those used by *Chemical Abstracts* and listed in the *Chemical Abstracts Service Source Index*. The abbreviations for the most frequently cited journal titles may be found in *The ACS Style Guide* or on the Web at http://www.cas.org/sent.html. For patents, and for journals that are not easily obtainable by most readers, a *Chemical Abstracts* citation should also be given.

2.2 Specialized Data

Data needed to document structure assignments, purity assessments, and other conclusions should be included in the manuscript or in the supporting information for publication. Referencing a link on an author's Web page, or stating that data will be provided to readers upon request, is not an acceptable alternative.

2.2.1 Synthesis Experiments. In reporting synthetic work, authors should include in the experimental section descriptions of new reactions and procedures, substantially modified or improved literature procedures, and key steps in multistep syntheses. Detailed descriptions of standard functional group transformations in multistep sequences (such as protection and deprotection steps), and characterization data for previously reported compounds should be included in the supporting information for publication. Procedures that were reported in the experimental section or supporting information of a previous publication should be cited but not reported in detail unless they have been modified.

If a synthesis procedure is used more than once, the experimental section should include only one detailed representative example, including the characterization data for the product; analogous examples (procedures and product characterization data) should be placed in the supporting information. New compounds reported in the supporting information are assigned Registry Numbers and are indexed by *Chemical Abstracts*, and known compounds prepared by new or improved methods are indexed, even if they are not mentioned in the experimental section or in the results and discussion.

Each paragraph describing a synthesis experiment should give the product's systematic name (see section 2.3.4) and the structure number assigned to the compound in the results and discussion; thereafter, the compound should be identified by its structure number. Use of abbreviations or molecular formulas for reagents and solvents, and of structure numbers rather than chemical names to identify starting materials and intermediates, is encouraged.

When a new or improved synthetic method is described, the yields reported in experimental examples, and yields used for comparison with previously reported methods, should represent amounts of isolated and purified products, rather than chromatographically or spectroscopically determined yields. Reactant quantities and product yields should be reported in both weight and molar units. When chromatographically or spectroscopically determined yields are reported in a table to document the scope or optimization of a synthetic transformation using a range of starting materials, reagents, or reaction conditions, the isolation and purification of the products for several representative examples should be reported in the experimental section or supporting information, and the isolated yields for those examples should be included in the table.

When flash chromatography is used for product purification, both the support and solvent should be identified. Details such as size or type of glassware, and numbers and volumes of extraction and wash solvents, should not be included unless they are critical to the outcome of an experiment.

Reports of syntheses conducted in microwave reactors must clearly indicate whether sealed or open reaction vessels were used and must document the manufacturer and model of the reactor, the method of monitoring the reaction mixture temperature, and the temperature reached or maintained in each experiment. Reporting a wattage rating or power setting is not an acceptable alternative to providing temperature data. *Manuscripts describing work done with domestic (kitchen) microwave ovens will be accepted only when the reported studies have been conducted at atmospheric pressure.*

2.2.2 Compound Characterization Data. The Journal upholds a high standard for compound characterization to ensure that compounds being added to the chemical literature have been correctly identified and can be synthesized in known yield and purity by the reported preparation, isolation, and purification methods. For all **new** compounds, evidence adequate to establish both *identity* and *degree of purity* (homogeneity) must be provided. Purity documentation must be provided for **known** compounds whose preparation by a new or improved method is reported. For combinatorial libraries containing more than 20 compounds, complete characterization data must be provided for at least 20 diverse members.

For known compounds synthesized by published methods as starting materials, the method of preparation and the literature data used to confirm the materials' identity should be cited, and the technique(s) used to determine the materials' purity should be reported. For known compounds prepared by new or modified synthetic reactions, listings of IR and NMR absorptions and MS peaks should appear in the manuscript only if they do not duplicate published data.

A completed **Compound Characterization Checklist** (see section 3.3.2) must be provided, even if only known compounds were prepared, to help editors and reviewers assess the thoroughness of the identity and purity documentation.

Identity

NMR Spectra. In most cases, ^{1}H and ^{13}C NMR resonances should be listed for each new compound; the solvent and instrument frequency should be identified. ^{13}C NMR peak shifts should be rounded off to the nearest 0.1 ppm except when greater precision is needed to distinguish closely spaced peaks. Hydrogen multiplicity (C, CH, CH_2, CH_3) information obtained from DEPT or 2D spectra should be included. If detailed peak assignments are made, the type of NOESY or COSY methods used to establish atom connectivities and spatial relationships should be identified in a General Experimental Methods paragraph. A copy of a well-resolved 1D ^{1}H NMR spectrum of every new compound, and a copy of a proton-decoupled 1D ^{13}C spectrum, if available, should be included in the supporting information for publication. In cases where structure assignments of complex molecules depend heavily on NMR data interpretation, copies of the 2D spectra should also be furnished.

HRMS and Elemental Analysis. For new compounds, either HRMS or combustion elemental analysis data should be reported to support the molecular formula assignment. HRMS data should include the molecular formula of the reported peak; the Found value should have an estimated uncertainty small enough to exclude alternative plausible formulas. Elemental analysis Found values for carbon, hydrogen, and nitrogen (if present) should be within 0.4% of the theoretical (Calcd) values for the proposed

formula. The inclusion of fractional molecules of solvent or water in the molecular formula to improve the fit of the data usually reflects incomplete purification of the sample. If the reported formula includes such a molecule, independent evidence for its presence (such as NMR peaks with appropriate chemical shifts) should be presented.

Biomacromolecules. The structures of biomacromolecules may be established by providing evidence about sequence and mass. Sequences may be inferred from the experimental order of amino acid, saccharide, or nucleotide coupling, from known sequences of templates in enzyme-mediated syntheses, or through standard sequencing techniques. Typically, a sequence will be accompanied by MS data that establish the molecular weight. Additional characterization and physical property data should be placed in the supporting information for publication unless they are important to the discussion.

Specific Rotation. Specific optical rotations should be reported for isolated natural products, enantiopure compounds, and enantioenriched isomer mixtures when sufficient sample is available. Specific rotations based on the equation $[\alpha] = (100 \cdot \alpha)/(l \cdot c)$ should be reported as unitless numbers as in the following example: $[\alpha]_D^{20}$ −25 (*c* 1.9, $CHCl_3$), where the concentration *c* is in g/l00 mL and the path length *l* is in decimeters. The units of the specific rotation, (deg·mL)/(g·dm), are implicit and are not included with the reported value. The compositions of configurational isomer mixtures should be reported as enantiomeric or diastereomeric ratios or fractions, rather than as enantiomeric or diastereomeric excess values.

Other Data. Only those IR absorptions diagnostic for major functional groups, and only those MS peaks used for structure assignment, should be included in the experimental section. Complete peak listings and other spectroscopic data may be reported in the supporting information for publication. A melting point *range* should be reported for all crystalline compounds.

Purity. Evidence for documenting compound purity may include one or more of the following:

(1) A standard 1D ^{1}H NMR spectrum (required for new compounds; see '***Identity***' above) or proton-decoupled ^{13}C NMR spectrum showing at most only trace peaks not attributable to the assigned structure. A copy of a spectrum with a signal-to-noise ratio sufficient to permit seeing peaks with 5% of the intensity of the strongest peak should be included in the supporting information for publication.

(2) Combustion elemental analytical values for carbon and hydrogen (and nitrogen, if present) agreeing with calculated values within 0.4%.

(3) Quantitative gas chromatographic analytical data for distilled or vacuum-transferred samples, or quantitative HPLC analytical data for materials isolated by column chromatography or separation from a solid support. The stationary phase, solvent (HPLC), detector type, and percentage of total chromatogram integration represented by the product peak should be reported. Alternatively, a copy of the chromatogram may be included in the supporting information for publication.

(4) Electrophoretic analytical data obtained under conditions that permit observing impurities present at the 5% level.

(5) For *known* solid compounds, a narrow melting point range that is in close agreement with a cited literature value.

The type of evidence appropriate for demonstrating a compound's purity will necessarily depend on the method of preparation, the compound's air and thermal stability, the complexity of its structure, the nature of reasonably likely impurities, and the amount of sample available. For example, combustion analysis would not be a good choice for the product of an isomerization reaction; a ^{1}H NMR spectrum would need to be supplemented with other evidence when reasonably likely impurities (including unreacted starting materials) do not have unique resonances or are NMR-silent (e.g., an inorganic salt). A narrow melting point range is not sufficient by itself to document the purity of a new compound. HRMS data may be used to support a molecular formula assignment *but cannot be used as a criterion of purity*.

2.2.3 Spectra. Reproductions of spectra will be published in the results and discussion section only when concise numerical summaries are inadequate for the discussion. Papers dealing primarily with interpretation of spectra, and those in which band shape or fine structure needs to be illustrated, may qualify for this exception. When presentation of spectra is essential, only the pertinent sections, prepared as figures (see section 2.5.6), should be included. Spectra used as adjuncts to the characterization of compounds should be included in the supporting information for publication.

2.2.4 Crystallographic Data. Only data and graphics vital to the discussion should be included in the results and discussion. If the data are used solely for confirming compound identity or stereochemistry, a statement in the results and discussion or experimental section that the assignment is supported by an X-ray crystallographic structure determination is usually sufficient.

Regardless of the level of detail of the discussion of the structure, a Crystallographic Information File (CIF) containing complete details of data collection, crystal and unit-cell parameters, structure solution and refinement, and tables of atomic coordinates and thermal parameters, bond lengths, bond angles, and torsion angles should be furnished in the supporting information for publication. Reflection intensity data (structure factor tables) should not be included. If more than one crystal structure is being reported, the CIF for each structure should be furnished as a separate file. *CIFs are required whether or not conventional text tables of crystallographic data are included in the supporting information, and whether or not the data have been deposited with a crystallographic database*. CIFs should be saved in text-only (plain ASCII) format and should be assigned file names that identify the structure number used in the manuscript and that include a ".cif" extension (e.g. 14.cif); they should not be combined with other types of supporting information files.

Before being submitted, CIFs should be checked using the free checkCIF data-validation utility on the Paragon Plus Web site at http://pubs.acs.org/paragonplus/tools/validate_cifs.html. Any reported syntax errors should be corrected. Copies of the final data-validation reports should be retained in case a reviewer or editor has a question about the data.

For structures refined anisotropically, a full-page size thermal ellipsoid plot should be furnished as a figure in the supporting information for publication; the probability level should be indicated if it is different from 50%. The numbering of the atoms should match that used in the CIF. Spherical-atom or wire-frame plots, packing diagrams, stereo views, and other graphics may also be included in the supporting information when appropriate.

2.2.5 Computational Data. The level of theory, specific program, basis set, and relevant input parameters should be identified when reporting computational studies. Complete details of computational methods and results, reported in sufficient detail to allow other researchers to repeat the computations, should be placed in the supporting information for publication. The data should include *Z*-matrices or Cartesian coordinates and computed total energies of target or optimized structures, along with any other absolute energy values used to calculate relative energies reported in the paper. Where applicable, the number of imaginary frequencies should be reported to identify stable structures and transition states. The inclusion of these data should be confirmed on the **Compound Characterization Checklist** (see section 3.3.2). Graphics that are not vital to the discussion should be placed in the supporting information for publication.

2.3 Manuscript Text

2.3.1 Writing Style and Language Usage. Clarity and conciseness are critical requirements for reports published in

the Journal. Authors should consult *The ACS Style Guide* for guidance on style, chemistry-related word-usage conventions, nomenclature, physical quantity symbols and units, abbreviations, grammar, capitalization, punctuation, and formatting of references. Spelling and use of periods and commas in numbers should conform to U.S. usage. *Any author who is not fully fluent in English is urged to obtain assistance with manuscript preparation from a colleague whose native language is English or from a professional technical editing service.* Manuscripts with extensive English usage or grammar deficiencies will not be forwarded to reviewers.

2.3.2 Manuscript Templates. *Notes* must be created or reformatted with the *JOC* double-column single-spaced Note template; they may not be longer than four pages. *Articles* may optionally be created with the Journal's double-spaced Article template. Manuscript templates and instructions for their use can be downloaded at http://pubs.acs.org/paragonplus/submission/joceah−select the appropriate Template link. The templates are available in several versions of Microsoft Word.

A template is used either by typing or copying-and-pasting text into pre-formatted sections of the document, or by applying the template's various styles to the individual sections of an existing manuscript created with a word-processor (or with a different journal's template). If the latter method is used, the manuscript's margins, page-size setting, and (for Notes but not Articles) double-column formatting must be reset following incorporation of the styles from the template; detailed instructions are furnished with the template.

Whether or not a template is used, all graphics and tables must be inserted into the manuscript near their first mention in the text; they should not be grouped at the end of the text or uploaded as separate files.

2.3.3 Text File Formatting

Manuscripts Created with a *JOC* Template (*including all Notes*). The fonts and formatting embedded in the template should not be altered.

Articles Not Created with a *JOC* Template. Articles may be prepared with Microsoft Word, Corel WordPerfect, or LaTeX; a list of versions compatible with the Paragon Plus manuscript submission system can be found at http://pubs.acs.org/paragonplus/submission/software.html. LaTeX users should follow guidance at http://pubs.acs.org/paragonplus/submission/tex.html. The entire Article manuscript file, including the abstract, experimental section, and references and footnotes, must be formatted for **single-column, double-spaced text**. Tables not created with the word-processor's table tool should also be double-spaced. 12-Point Times, Times New Roman, Helvetica, Arial, or Courier fonts should be used for the text of the manuscript to minimize font-embedding problems when the word-processor file is converted to the PDF and HTML versions seen by the reviewers.

All Manuscripts

Fonts and Typography. The Symbol font (rather than the normal text font) must be used for Greek letters and mathematical symbols. The single-character symbol for degrees Celsius found in some fonts may not convert correctly to PDF and should not be used; instead, the degree sign in Symbol font should be followed by the capital letter C in the normal text font. The letters O, l, and x should not be substituted for the numerals 0 and 1 and the multiplication symbol ×. The 'en' dash (−) rather than the hyphen (-) should be used for the minus sign in all negative quantities.

Page Numbering. **The pages must be consecutively numbered** using the word processor's page-numbering feature. Page numbers should be positioned sufficiently far from the edges of the page that they will not be cut off when the PDF version is printed on U.S. letter-size paper.

Formatting and Page-Size Setting. Automatic hyphenation should be disabled, and line returns ("Return" or "Enter" key) should be used only at the end of paragraphs and section headings. Before the manuscript text word-processor file is saved, the paper-size setting in the word-processor's Page Setup menu must be set to U.S. Letter (8.5 × 11 in., 22 × 28 cm). If the A4 or another setting is used, page numbers or lines of text may be lost when an editor or reviewer prints the PDF file on U.S. letter-size paper.

Saving the File. When saving the manuscript file, the file format should not be changed from the word processor's default document file type. The file name should include a three-letter file extension (".doc" for Word; ".wpd" for WordPerfect), even if the manuscript is created on a non-Windows computer. An exception is that if a non-Western version of a word processor is used, the file should be saved and submitted in Rich Text Format with a ".rtf" file name extension. The word-processor file must not be password-protected and must not contain comments, tracked changes, or color-highlighted text.

2.3.4 Nomenclature. Authors should furnish a correct systematic name, following International Union of Pure and Applied Chemisry (IUPAC) conventions, for each compound whose preparation is reported in the experimental section or supporting information. Complex compounds with lengthy or unwieldy names may be referred to by their functional class and structure number (e.g., ketone **23**) elsewhere in the text. IUPAC guides to organic and biochemical nomenclature are available on the Web at http://www.acdlabs.com/iupac/nomenclature. For certain specialized classes of compounds such as steroids, peptides, carbohydrates, and cyclophanes, the name should conform to the nomenclature conventions generally accepted for that class. The use of italics, capitals, small capitals, hyphens, parentheses, and square brackets for positional, configurational, and stereochemical prefixes and identifiers should conform to *The ACS Style Guide*.

2.3.5 Abbreviations, Physical Quantity Symbols, and Units. Authors are encouraged to use abbreviations and acronyms to conserve space. The Journal's list of standard abbreviations and acronyms is included in section 4 of these Guidelines. Nonstandard abbreviations and acronyms must be defined the first time they are used. The use of abbreviations should be consistent throughout the manuscript text, tables, and graphics. For example, either CH_3 or Me may be used for "methyl", but not both. The use of abbreviations and acronyms in the title and abstract should be avoided.

Single-letter symbols for physical quantities should be italicized (e.g., c, E_a, J, m/z, $t_{1/2}$). The International System of Units (SI units) should generally be used, but authors may also use common non-SI metric units such as Å, cal, cm^{-1}, eV, g, Hz, L, ppm, and °C.

2.4 Tables

The use of tables is encouraged for presenting data in a space-efficient manner. **Tables must be inserted in the manuscript word-processor file near their first mention in the text**; they should not be grouped together at the end of the text. Tables should be created with the word processor's table-formatting feature. Each data entry should be placed within its own table cell; tabs and line returns should not be used within cells. Whenever possible, structure numbers should be used in tables rather than small chemical structure graphics. If a table-formatting feature is not available, adjacent columns should be separated with tabs rather than spaces, and a line return should be inserted at the end of each row. Tables should be prepared at the actual sizes at which they are intended to appear in the printed edition of the Journal, in either single column (up to 3.3 in., 8.4 cm) or double column (up to 7.0 in., 17.8 cm) width. Arrangements that leave many columns only partially filled should be avoided.

Above each table should be typed, in boldface characters, a sequential Arabic table number and a short descriptive title (e.g., **Table 3. Strain Energies of Substituted Spiropentanones**). The title, together with the individual column and row headings and footnotes, should make the table self-explanatory; titles and

footnotes containing "see text" should be avoided. If the word-processor's table tool is used, the table number, title, and any footnotes should not be placed in table cells but should be typed above or below the table. No collected list of all the table titles should be included at the end of the manuscript.

Footnotes for tables should be given lowercase italic letter designations and should be cited in the table with lowercase italic superscripted letters. The sequence of letters should proceed by row, and from left to right within any rows having more than one footnote. If a reference is cited both in the text and in a table, the lettered footnote in the table should cite the text reference's number.

2.5 Graphics

2.5.1 General Requirements. All graphics (illustrations) must be prepared in digital format and inserted into the manuscript word-processor file near their first mention in the text; they should not be grouped together at the end of the text or uploaded as separate 'Graphic for manuscript' files. Graphics intended to appear in black-and-white or grayscale should not be submitted in color. When areas in a graphic created with a graphics program need to be shaded or filled in, parallel lines or crosshatching, rather than gray shading, should be used whenever possible to allow the graphic to be processed as line art rather than as grayscale art. Additional guidance on creating graphics for manuscripts may be found in *The ACS Style Guide*, 3rd edition, chapters 15 (Figures) and 17 (Chemical Structures).

2.5.2 Color. The editors encourage the use of color in manuscript graphics and in the table of contents graphic when it is important for clarity of presentation. Although there is no charge for inclusion of color illustrations in the manuscript, paper reprints containing color graphics have a supplemental color charge of $100 per 100 copies. There are no restrictions on the use of color in the supporting information. In selecting colors for illustrations, authors should keep in mind that many readers will print the published paper on monochrome printers or will receive black-and-white copies from document providers.

2.5.3 Quality. Because the graphics inserted into the manuscript are used for production, the quality of the graphics published in the Journal depends on the quality of the graphic images provided by authors. *Chemical structure graphics and figures can be moved and rescaled by the Journal production staff if necessary, but they cannot be otherwise modified or enhanced to correct problems or to improve their appearance.* Digital graphics in the *manuscript* should have the following minimum resolution:

Black-and-white line art	1200 dpi
Grayscale art	600 dpi
Color art	300 dpi

For graphics in the *supporting information*, which is made available to readers only via the Internet, a resolution of 150 dpi is usually adequate.

For uniformity of appearance, all the graphics of the same type (e.g., chemical structures, graphs, spectra) should share a common graphic style and a common lettering font and size. Lettering and lines should be of uniform density. Arial or Helvetica font is preferred for lettering; the size should be at least 5.0 points. Lines should be no thinner than 1.0 point.

2.5.4 Inserting Graphics into the Manuscript. For manuscripts created with a word-processor program, each graphic should be copied from the graphics program and pasted into its appropriate location in the manuscript text file. To allow pasted graphics to be positioned without overlapping nearby text, Microsoft Word users may need to deselect the "Float over text" picture format setting (Word 97 and 98) or select "In line with text" as the wrapping style (Word 2000, 2001, and later versions). If a pasted graphic needs to be resized or relabeled, it should be re-edited *in the graphics program* and pasted again into the word-processor file (rather than modified within the word-processor program). *No page-layout or graphics-placement instructions should be typed into the text file*.

For manuscripts created with LaTeX, the guidelines on the Paragon Plus Web site at http://pubs.acs.org/paragonplus/submission/tex.html should be consulted.

2.5.5 Chemical Structure Graphics. *Structures* are chemical structural formula line drawings used in schemes, equations, and structure blocks. A *scheme* depicts, with multiple reaction arrows, a series of chemical transformations among several structures. It may have vertical and diagonal as well as horizontal arrows, is identified with a sequential Arabic boldface numeral, and may have a short descriptive title (e.g., **Scheme 2. Synthesis of 10**). The scheme number and optional title are positioned *above* the scheme and should be typed at the appropriate location in the manuscript text word-processor file, not in the graphics program used to create the scheme. No collected list of all the scheme titles should be included at the end of the manuscript.

In reaction schemes, abbreviations for reagents, solvents, and reaction conditions should be placed above the horizontal reaction arrows or adjacent to the vertical arrows; only if there is insufficient space should they be placed in footnotes below the scheme (with the footnotes typed into the manuscript text file and keyed to lowercase letters placed above or next to the arrows). It is not necessary to indicate reagents and conditions in detail, since this information should be available in the experimental section, in the supporting information, or in a cited reference.

An *equation* illustrates simpler transformations with structures and horizontal reaction arrows in a single line, or expresses a relationship among mathematical or physical quantities. It is identified with a sequential Arabic numeral in parentheses, e.g. (4), flush with the right margin, has no title or footnotes, and is cited in the text with "eq" followed by the numeral.

A *structure block* is a group of chemical structures that are placed together for efficient use of space. Structure blocks have neither numbers nor titles, and the structures are not linked with reaction arrows.

Formatting. Structures should be produced with a drawing program such as ChemDraw. Authors using recent versions of ChemDraw will find the necessary formatting parameters incorporated as the "ACS Document 1996" option in the Apply Document Settings menu. In ChemDraw Preferences, "cm" should be chosen as the units, and the tolerance should be set at 3 pixels. For Macintosh versions of ChemDraw, the following Preferences options should be enabled: 'Include PostScript', 'Include ChemDraw Laser Prep', and 'Optimize Pictures for High-Resolution Non-PostScript Printing'. Authors using older versions of ChemDraw or other drawing programs should select settings as close as possible to the following:

Drawing Settings	
chain angle	120°
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.)
Text Settings	
font	Arial or Helvetica
size	10 pt

Dimensions and Layout. Chemical structure graphics should be prepared and inserted into the manuscript at the actual sizes at which they are intended to appear in the printed edition of the Journal, in either single column (up to 3.3 in., 8.4 cm) or double column (up to 7.0 in., 17.8 cm) width. Structures, arrows, and structure numbers should be arranged to make maximum use of the available one- or two-column width and to occupy the minimum height necessary. Only one-column-wide schemes, structure blocks, and equations can be placed at a preferred

location in the printed edition, usually near their first mention in the text; two-column-wide graphics are generally placed at the top of a page.

Labeling of Structures. Within structure blocks, equations, and schemes, the individual structures should be numbered with boldface Arabic numerals ("structure numbers"), in Arial or Helvetica font, in the order in which the compounds are first mentioned in the text. To avoid the need to repeat similar structures, boldface lowercase letters may be used immediately following the numerals (e.g., **5a**, **5b**) to distinguish variants that differ only in the identity of substituents (indicated with $\mathbf{R^1}$, $\mathbf{R^2}$, **X**, etc.). No structure should appear more than once; a compound that appears in several schemes or equations should be designated with its structure number alone after its first appearance as a structure. Where needed, numbers such as ring position indicators or NMR chemical shifts, or other markings such as double-headed arrows showing NOE correlations, may be included in structures.

2.5.6 Figures. Diagrams, graphs, spectra, photographs, and all other types of illustrations are presented in the Journal as figures with captions. Blocks of structures and reaction schemes should not be designated as figures. Figures should be prepared and inserted into the manuscript at the actual sizes at which they are intended to appear in the printed edition of the Journal, in either single column (up to 3.3 in., 8.4 cm) or double column (up to 7.0 in., 17.8 cm) width. During production of the printed edition, figures are placed at the top of a journal column or page.

Figures are consecutively numbered with boldface Arabic numerals and have brief descriptive captions. The figure number and caption should be typed in the manuscript word-processor file directly *below* the figure (rather than included in the graphic). The caption should identify the content of the figure and should be understandable without reference to the text. If a figure has several parts, the individual parts should be labeled (a), (b), etc., and each part identified in the caption. No collected list of the figure captions should be included at the end of the manuscript. The key to symbols used in a figure (for example, for marking experimental points in a graph) should be included in the figure itself whenever possible.

2.5.7 Table of Contents Graphic. A graphic must be included in each manuscript that will appear both (1) in the table of contents (TOC) of the Journal issue in which the Article or Note is published and (2) in the published paper immediately above the abstract. This graphic should capture the reader's attention and, in conjunction with the manuscript's title, should give the reader a quick visual impression of the type of chemistry described in the paper. *The TOC graphic should not exactly duplicate a graphic appearing within the text of the manuscript.* Structures in the TOC graphic should be constructed as specified in section 2.5.5 ('Chemical Structure Graphics'). Annotations should be limited to labels for compounds, reaction arrows, and figures. The use of standard abbreviations and unambiguous molecular formulas for common substituents, reagents, and solvents is encouraged. The TOC graphic may be up to 3.5 in. (9.0 cm) wide and 1.4 in (3.5 cm) tall. It should be copied and inserted between the corresponding author's e-mail address and the abstract.

2.6 Supporting Information for Publication

Where the term "supporting information" is used in these Guidelines, it refers to the supporting information for publication and not to the supporting information for review only (section 3.3.4). The technical content of the supporting information is discussed in several sections above: 2.1.7 ('Results and Discussion'), 2.1.9 ('Experimental Section'), and 2.2 ('Specialized Data'). This section describes the mechanics of preparing the supporting information for submission.

A wide range of electronic formats is supported; a complete list can be found on the Paragon Plus Web site at http://pubs.acs.org/paragonplus/submission/software.html. They include formats for color illustrations, rotatable molecular models, animations, and videos.

All text and graphics (including spectra) should be combined into a single word-processor or PDF file. If submission as a single file is not possible, then all files of the same file type should be combined. The individual files should be given informative file names (for example, Characterization_data.doc and NMR_spectra.pdf). **Authors should not furnish multiple image files each containing a single spectrum or chromatogram.** The size of any single file is limited to 5 MB. During submission, files with text and graphics submitted in word-processor format will be automatically converted to PDF files for posting on the supporting information Web server. Authors should not submit both word-processor and PDF versions of the same supporting information file. Crystallographic information files (CIFs) should be uploaded separately from other types of files.

Text in the supporting information should adhere to the same formatting and font requirements as the manuscript text (see section 2.3.3). The graphics must meet the same quality standards as the graphics in the manuscript. Incorporating images created or saved at resolutions higher than 150 dpi will not substantially improve the appearance of graphics in the Web-based supporting information but will result in large file sizes that inconvenience reviewers, editors, and future readers with long download times. Spectra should be at least a half page in size, be in sharp focus, have dark unbroken lines, and be labeled with both a structure number (or table-entry number) and a small graphic of the structure. Axis labels and scales, peak frequencies or chemical shifts, and all other text and numerical information must be clearly legible. If the manuscript reports the preparation of a compound under more than one set of experimental conditions, the spectrum's labeling or caption must indicate which conditions produced the sample whose spectrum is illustrated; in many cases this can be accomplished by providing a table-entry number. For NMR spectra, the solvent and instrument frequency should be indicated on the spectra or in the supporting information's table of contents (see below). Informative captions for figures other than spectra should appear directly below the figures. There are no restrictions on the use of color in supporting information graphics.

All the pages of supporting information files containing text and graphics must be consecutively numbered S1, S2, S3, ... *The first page (page S1) must be a title page containing the title of the manuscript, the names of the authors, and a table of contents with the page numbers of the included data.* The requirements for providing a title page with table of contents and for numbering the pages do not apply to crystallographic data submitted as CIFs or to nontext files.

The supporting information for publication is not edited during Journal production and will appear on the archival Web server exactly as submitted. Authors should be aware that references that are included in the supporting information but not in the manuscript are not indexed by *Chemical Abstracts* and *Science Citation Index.*

A Supporting Information Available statement identifying the type of supplementary material being furnished must be inserted in the text of the manuscript immediately before the references and footnotes (see section 2.1.11). *The manuscript cannot be forwarded for review or publication if this statement is missing.*

3 Submitting the Manuscript

3.1 Using the Paragon Plus Web Site

The manuscript and other submission items (see section 3.3) should be uploaded at the ACS Paragon Plus Web site at http://paragonplus.acs.org. The Journal does not accept mailed hard-copy manuscripts or manuscripts submitted by e-mail.

Before submitting a manuscript, the corresponding author (or a designee who will be making the submission) must register

on the Paragon Plus Web site. Once registered, an author may submit manuscripts to any ACS journal and may check the processing status of submitted manuscripts. Registration is not required to access information about preparing and submitting manuscripts. The Web site's security features limit access to a submitted manuscript to the editorial offices and to those reviewers to whom that manuscript is assigned.

During the submission process, the author will be asked to enter the names, institutions, and e-mail addresses of at least five researchers qualified to act as reviewers.

3.2 Priority Processing

Manuscripts that are complete and that adhere to the requirements in these Guidelines will receive priority for processing by the Editor-in-Chief's office and for assignment to an associate editor. The specific requirements that need to be met to qualify for priority processing are listed in section 5 of these Guidelines.

If required material such as compound purity documentation, crystallographic data, or other supporting information is missing, of if a pre-review revision is necessary because the manuscript does not conform to the Journal's formatting requirements or is missing a required experimental section or Supporting Information Available statement, the author will be given 14 days to furnish a revised submission. *The "Received" date will be changed to the date on which the complete, properly formatted submission is received in the Editor-in-Chief's office.*

3.3 Additional Items to be Submitted

The names of all files uploaded on Paragon Plus should include a three-letter file extension (for example, ".doc" for Microsoft Word, or ".pdf" for Portable Document Format), even if the manuscript is created and submitted on a non-Windows computer. As each file is uploaded, the appropriate file designation (for example, 'Manuscript text with embedded graphics', 'Compound Characterization Checklist', 'Supporting Information for Publication', or 'Supporting Information for Review Only') should be selected from the menu on the file-upload Web page.

3.3.1 Cover Letter. A cover letter must accompany every manuscript. The cover letter should include the corresponding author's name, postal and e-mail addresses, and telephone and fax numbers; the title of the manuscript; and a brief paragraph pointing out the significance of the reported work. If the manuscript has not been previously submitted to this Journal, a preference for the manuscript to be assigned to a particular associate editor may be indicated.

Article Based on a Preliminary Report. If the manuscript is an extension of a published or "in-press" letter or communication, the preliminary report must be mentioned in the cover letter and cited in the manuscript, and a copy of the report *and any associated supporting information* must be uploaded as supporting information for review only (see section 3.3.4).

Previous Submission. If substantially the same manuscript has been previously submitted to this Journal or to another ACS journal, the cover letter must mention the earlier submission. Copies of all of the reviews should be appended to the cover letter file (not uploaded as supporting information), and the cover letter should include a detailed explanation of any revisions, whether or not they were made in response to reviewer and editor comments.

Permission for Use of Work of Others. Copies of letters or e-mail messages of permission are required when authors cite personal communications with, unpublished results from, or "in-press" papers by researchers who are not coauthors. This requirement does not apply to data obtained from commercial or in-house service laboratories.

A manuscript incorporating text, tables, or figures from a copyrighted publication must be accompanied by a copy of a letter or message from the copyright holder identifying the material and granting permission to reproduce it. Permission is not needed when the material is from a paper by one or more of the coauthors published in an ACS journal.

The permission letters or messages should be appended to the cover letter file. If this cannot be done, copies marked with the assigned manuscript number should be faxed or e-mailed to the associate editor who is coordinating the peer review.

3.3.2 Compound Characterization Checklist. Manuscripts that report the characterization of new or previously reported compounds or the results of theoretical computations must be accompanied by a completed Compound Characterization Checklist. The Checklist will be provided to the reviewers to help them assess the overall thoroughness of the characterization of compounds and the reporting of computational results.

The Checklist form is available as a Microsoft Excel file on the Paragon Plus Web site at http://pubs.acs.org/paragonplus/submission/joceah−select the Compound Characterization Checklist link. The form should be completed on-screen and saved with a ".xls" file extension. Alternatively, the form may be photocopied from the first printed Journal issue of the current year, completed by hand, scanned, and saved with an appropriate image file extension.

3.3.3 Supporting Information for Publication. The technical content and formatting of supporting information files submitted with the manuscript are discussed in section 2 ('Preparing the Manuscript and Supporting Information for Publication').

3.3.4 Supporting Information for Review Only. If the manuscript is an extension of a published or "in-press" letter or communication, a copy of the preliminary report *and any supporting information associated with it* must be uploaded as a supporting information for review only file. When related work is cited but is not available to editors and reviewers because it is "in press" or "submitted for publication", a copy of the cited manuscript should be provided in this manner. When an author requests "back-to-back" publication of related manuscripts submitted at the same time, each manuscript should include a copy of the other as supporting information for review only. Authors may upload as review-only files any additional material not intended for publication that they wish the editors and reviewers to see. (Any material the author wishes the editor *but not the reviewers* to see should be either appended to the cover letter file or uploaded as 'Other files for Editors only'.)

3.3.5 Copyright Status Form. A properly completed and signed Copyright Status Form must be provided for each submitted manuscript. The form may be downloaded from the Paragon Plus Web site at http://pubs.acs.org/paragonplus/copyright/ and either printed and completed by hand, or completed on-screen, printed, and signed by hand. Alternatively, the form may be photocopied from the first printed Journal issue of the current year. The signed form should be scanned, and the image file uploaded as a 'Completed and Signed Copyright Form' at the time of manuscript submission. If a manuscript is not accepted for publication, is withdrawn by the author, or is inactivated by the editor, the transfer of the copyright to the ACS is automatically canceled.

The supporting information for publication associated with an accepted and published manuscript is considered part of the publication and is covered by the copyright assignment in the Copyright Status Form.

3.4 Revising the Manuscript

In revising a manuscript following peer review or editor evaluation, the author should address any technical concerns raised by the editor and reviewers. If substantial changes need to be made in content or interpretation, it is appropriate for the author to obtain the concurrence of the other coauthors. Corrections noted in the editor's letter or on an accompanying Revision Request List should also be accommodated. *For Notes, the changes must be made without exceeding the four-page length limit.* The revision should be checked for consistent notation and for consecutive numbering of structures, schemes,

equations, figures, tables, and references. References should be reverified, and the status of any "submitted for publication" and "in press" manuscripts, and of any references cited as *Articles ASAP* at the time of manuscript submission, should be updated. The revised manuscript file must not contain comments, tracked changes, or color-highlighted text.

The revision must be uploaded on the Paragon Plus Web site as a revised submission, **not as a new manuscript**. It may not be submitted by e-mail or mailed as hardcopy. The original manuscript file must be removed before the revised version is uploaded. New or replacement supporting information files can be added during revision; any files that are being replaced with updated versions should be removed. If supporting information for publication is being added to a manuscript that previously had none, a Supporting Information Available statement (see section 2.1.11) must be added to the manuscript text file. Changes to the manuscript and to the supporting information for publication, whether or not made in response to the reviewer and editor comments, should be pointed out in the "Response to Decision Letter" section of the revision-submission Web page. Any change in the manuscript's title, abstract, or list of coauthors must be disclosed.

If the first revision requested following peer review is not returned to the editor within 45 days, and the author has not made alternative arrangements with the editor for completion of the revision, the manuscript will be inactivated and removed from the author's Paragon Plus home page. An inactivated manuscript that is subsequently reactivated at the author's request will be assigned a new "Received" date.

3.5 Page Proofs

The page proofs and a reprint order form will be provided to the corresponding author as a Web link. An author who wishes to receive hardcopy proofs should contact the Editor-in-Chief's office. Corresponding authors who authorize a coauthor to correct the proofs are reminded that any order for paper reprints (see section 3.6) must be placed at the time the proof corrections are submitted.

The author should return a detailed list of any needed corrections. Only typographic corrections and other minor changes may be made at the page proof stage. Any substantive changes will require editorial approval and may delay publication. Changes to the supporting information for publication cannot be made as part of proof correction.

3.6 E-prints and Reprints

Under the ACS Articles on Request policy, the Society will provide (free of charge) to all contributing authors a unique URL within the ACS Web site that they may e-mail to colleagues or post on external Web sites. These author-directed links are designed to facilitate distribution of an author's published work to interested colleagues. The ACS Articles on Request policy allows 50 downloads within the first year after publication and unlimited access via the same author-directed links 12 months after publication.

The ACS AuthorChoice option establishes a fee-based mechanism for authors or their research funding agencies to sponsor the open availability of their articles on the Web at the time of online publication. Under this policy, the ACS as copyright holder will enable unrestricted Web access to a contributing author's publication from the Society's Web site in exchange for a fixed payment from the sponsoring author. ACS AuthorChoice will also enable participating authors to post electronic copies of published articles on their own personal Web sites and institutional repositories for noncommercial scholarly purposes and allow immediate open access to an article as soon as it is published on the ACS Web site. For more details on ACS AuthorChoice, please visit http://pubs.acs.org/4authors/authorchoice/.

For paper reprints, the reprint order form and purchase order or check should be sent prior to the publication date to Cadmus Reprints, P.O. Box 751903, Charlotte, NC, USA 28275-1903. Reprints will be shipped within two weeks after the printed issue date. Neither the Editors nor the Washington ACS Office keeps a supply of reprints; requests for single copies of papers should be addressed to the corresponding author of the paper concerned.

3.7 Additions and Corrections

If an error or omission of consequence is discovered in a paper published in the Journal, the corresponding author should contact the Editor-in-Chief (e-mail: joc@chem.utah.edu) for instructions on submitting an addition or correction. Acceptance of an addition or correction is subject to approval by the Editor-in-Chief.

3.8 For Additional Help

The Paragon Plus Web site has links to detailed information about manuscript submission. Questions about manuscript preparation and online manuscript submission should be e-mailed to the Journal Help Desk at paragonplus@acs.org. Questions about manuscript requirements specific to *The Journal of Organic Chemistry* may be e-mailed to the Editor-in-Chief's office at joc@chem.utah.edu.

4 Standard Abbreviations and Acronyms

α	observed optical rotation in degrees
[α]	specific rotation [expressed without units; the units, (deg·mL)/(g·dm), are understood]
Å	angstrom(s)
Ac	acetyl
acac	acetylacetonate
ADP	adenosine 5′-diphosphate
AIBN	2,2′-azobisisobutyronitrile
AM1	Austin model 1
AMP	adenosine 5′-monophosphate
anhyd	anhydrous
AO	atomic orbital
aq	aqueous
Ar	aryl
atm	atmosphere(s)
ATP	adenosine 5′-triphosphate
ATPase	adenosinetriphosphatase
av	average
9-BBN	9-borabicyclo[3.3.1]nonyl
9-BBN-H	9-borabicyclo[3.3.1]nonane
Bn, Bzl	benzyl
bpy	2,2′-bipyridyl
BOC, Boc	*tert*-butoxycarbonyl
bp	boiling point
br	broad (spectral)
Bu, *n*-Bu	normal (primary) butyl
s-Bu	*sec*-butyl
t-Bu	*tert*-butyl
Bz	benzoyl (not benzyl)
B3LYP	3-parameter hybrid Becke exchange/Lee−Yang−Parr correlation functional
°C	degrees Celsius
calcd	calculated
cAMP	adenosine cyclic 3′,5′-phosphate
CAN	ceric ammonium nitrate
CASSCF	complete active space self-consistent field
CASPT2	complete active space with second-order perturbation theory
cat	catalytic
CBZ, Cbz	benzyloxycarbonyl
CC	coupled cluster
CD	circular dichroism
cDNA	complementary deoxyribonucleic acid
c-Hex, *c*-C_6H_{11}	cyclohexyl
CI	chemical ionization; configuration interaction
CIDNP	chemically induced dynamic nuclear polarization
cm	centimeter(s)
cm^{-1}	wavenumber(s)
cod	1,5-cyclooctadiene
compd	compound
concd	concentrated
concn	concentration
COSY	correlation spectroscopy
cot	1,3,5,7-cyclooctatetraene
Cp	cyclopentadienyl
m-CPBA	*meta*-chloroperoxybenzoic acid
CV	cyclic voltammetry
δ	chemical shift in parts per million downfield from tetramethylsilane
d	day(s); doublet (spectral); deci
d	density
DABCO	1,4-diazabicyclo[2.2.2]octane
dansyl	5-(dimethylamino)-1-naphthalenesulfonyl
DBN	1,5-diazabicyclo[4.3.0]non-5-ene
DBU	1,8-diazabicyclo[5.4.0]undec-7-ene
DCC	*N*,*N*′-dicyclohexylcarbodiimide
DCE	1,2-dichloroethane
DDQ	2,3-dichloro-5,6-dicyano-1,4-benzoquinone
DEAD	diethyl azodicarboxylate
DEPT	distortionless enhancement by polarization transfer
DFT	density functional theory
DIBALH	diisobutylaluminum hydride
DMA	dimethylacetamide
DMAP	4-(*N*,*N*-dimethylamino)pyridine
DMDO	dimethyldioxirane
DME	1,2-dimethoxyethane
DMF	dimethylformamide
DMPU	1,3-dimethyl-3,4,5,6-tetrahydro-2(1*H*)-pyrimidinone
DMSO	dimethyl sulfoxide
DMTrCl	4,4′-dimethoxytrityl chloride
DNA	deoxyribonucleic acid
DPS	*tert*-butyldiphenylsilyl
dr	diastereomeric ratio (not diastereomeric excess)
DTT	dithiothreitol
E1	unimolecular elimination
E2	bimolecular elimination
ED_{50}	dose that is effective in 50% of test subjects
EDTA	ethylenediaminetetraacetic acid
EI	electron impact
EPR	electron paramagnetic resonance
eq	equation
equiv	equivalent
er	enantiomeric ratio (not enantiomeric excess)
ESI	electrospray ionization
Et	ethyl
FAB	fast atom bombardment
FD	field desorption
FID	flame ionization detector; free induction decay
Fmoc	9-fluorenylmethoxycarbonyl
FT	Fourier transform
g	gram(s); prefix to NMR abbreviation denoting gradient-selected (e.g., gCOSY, gHMQC)
GC	gas chromatography
GTP	guanosine 5′-triphosphate
h	hour(s)
HF	Hartree−Fock
HMBC	heteronuclear multiple bond correlation
HMPA	hexamethylphosphoric triamide (hexamethylphosphoramide)
HMQC	heteronuclear multiple quantum correlation
HOMO	highest occupied molecular orbital
HPLC	high-performance liquid chromatography
HRMS	high-resolution mass spectrometry
HSQC	heteronuclear single quantum correlation
Hz	hertz
ICR	ion cyclotron resonance
INDO	intermediate neglect of differential overlap
IP	ionization potential
IR	infrared
J	coupling constant (in NMR spectrometry)
k	kilo
K	kelvin(s) (absolute temperature)
L	liter(s)
LAH	lithium aluminum hydride
LCAO	linear combination of atomic orbitals
LD_{50}	dose that is lethal in 50% of test subjects
LDA	lithium diisopropylamide; local density approximation
LFER	linear free energy relationship
LHMDS	lithium hexamethyldisilazane, lithium bis(trimethylsilyl)amide
lit.	literature value (abbreviation used with period)
LTMP	lithium 2,2,6,6-tetramethylpiperidide
LUMO	lowest unoccupied molecular orbital
μ	micro
m	multiplet (spectral); meter(s); milli
M	molar (moles per liter); mega
M^+	parent molecular ion
MALDI	matrix-assisted laser desorption ionization
max	maximum
MCD	magnetic circular dichroism
MCR	multicomponent reaction

MCSCF	multi-configuration self-consistent field
MD	molecular dynamics
Me	methyl
MEM	(2-methoxyethoxy)methyl
Mes	2,4,6-trimethylphenyl (mesityl) [not methylsulfonyl = mesyl]
MHz	megahertz
min	minute(s); minimum
mM	millimolar (millimoles per liter)
MO	molecular orbital
mol	mole(s); molecular (as in mol wt)
MOM	methoxymethyl
mp	melting point
MP	Møller−Plesset perturbation theory
MRCI	multi-reference configuration interaction
mRNA	messenger ribonucleic acid
Ms	methylsulfonyl (mesyl)
MS	mass spectrometry
MTBE	methyl *tert*-butyl ether
MW, mol wt	molecular weight
m/*z*	mass-to-charge ratio (not *m*/*e*)
N	normal (equivalents per liter)
NAD^+	nicotinamide adenine dinucleotide
NADH	reduced NAD
NBO	natural bond orbital
NBS	*N*-bromosuccinimide
NCS	*N*-chlorosuccinimide
NICS	nucleus-independent chemical shift
nm	nanometer(s)
NMO	*N*-methylmorpholine-*N*-oxide
NMP	*N*-methylpyrrolidone
NMR	nuclear magnetic resonance
NOE	nuclear Overhauser effect
NOESY	nuclear Overhauser effect spectroscopy
NRT	natural resonance theory
Nu	nucleophile
obsd	observed
OD	optical density
ORD	optical rotary dispersion
PCC	pyridinium chlorochromate
PDC	pyridinium dichromate
PES	photoelectron spectroscopy
Ph	phenyl
piv	pivaloyl
pm	picometer(s)
PM3	parametric method 3
PPA	poly(phosphoric acid)
ppm	part(s) per million
PPTS	pyridinium *para*-toluenesulfonate
Pr	propyl
i-Pr	isopropyl
PT	perturbation theory
PTC	phase-transfer catalysis
py	pyridine
q	quartet (spectral)
QSAR	quantitative structure−activity relationship
RCM	ring-closure metathesis
redox	reduction−oxidation
rel	relative
R_f	retention factor (in chromatography)
RHF	restricted Hartree−Fock
ROESY	rotating frame Overhauser effect spectroscopy
ROMP	ring-opening metathesis polymerization
rRNA	ribosomal ribonucleic acid
rt	room temperature
s	singlet (spectral); second(s)
SAR	structure−activity relationship
SCF	self-consistent field
SEM	scanning electron microscopy
SET	single electron transfer
S_N1	unimolecular nucleophilic substitution
S_N2	bimolecular nucleophilic substitution
S_N'	nucleophilic substitution with allylic rearrangement
SOMO	single-occupied molecular orbital
t	triplet (spectral)
TBAB	tetrabutylammonium bromide
TBAC	tetrabutylammonium chloride
TBS	*tert*-butyldimethylsilyl
TBHP	*tert*-butyl hydroperoxide
TCA	trichloroacetic acid
TCNE	tetracyanoethylene
TDDFT	time-dependent density functional theory
TEAB	tetraethylammonium bromide
temp	temperature
Tf	trifluoromethanesulfonyl (triflyl)
TFA	trifluoroacetic acid
TFAA	trifluoroacetic anhydride
THF	tetrahydrofuran
THP	tetrahydropyran-2-yl
TIPS	triisopropylsilyl
TLC	thin-layer chromatography
TMAI	tetramethylammonium iodide
TMEDA	*N*,*N*,*N*′,*N*′-tetramethyl-1,2-ethylenediamine
TMS	trimethylsilyl; tetramethylsilane
TOF	time-of-flight
Tr	triphenylmethyl (trityl)
tRNA	transfer ribonucleic acid
t_R	retention time (in chromatography)
Ts	*para*-toluenesulfonyl (tosyl)
TS	transition state
UHF	unrestricted Hartree−Fock
UV	ultraviolet
VCD	vibrational circular dichroism
vis	visible
vol	volume
v/v	volume per unit volume (volume-to-volume ratio)
wt	weight
w/w	weight per unit weight (weight-to-weight ratio)
ZINDO	Zerner parametrization of intermediate neglect of differential overlap

5 Priority Processing Requirements

To qualify for priority in the initial processing and assignment to an associate editor, a manuscript needs to meet the minimum formatting and completeness requirements listed below. Most of these requirements have been established to facilitate the job of the reviewers and editors. Evaluation of a manuscript not meeting these requirements will be delayed while the Journal office requests a pre-review revision. The manuscript will be assigned a new "Received" date when the revision is received.

Manuscript File

- A *Note* must be created (or reformatted) using the single-spaced *JOC* Note template and must be shorter than four pages.
- An *Article* must be entirely double-spaced.
- The references and any footnotes must be grouped into a single list at the end of the manuscript file.
- The manuscript's graphics and tables must be inserted into the text near their first mention. They should not be grouped together at the end of the manuscript or uploaded as separate files.
- The manuscript, whether an Article or Note, must include a separate Experimental Section, even if most of the experimental details are presented in the supporting information for publication. (This requirement does not apply to reports of purely theoretical studies.)
- The manuscript and supporting information for publication files must be free of font and graphics-quality problems.
- The manuscript must not have extensive English usage or grammar deficiencies.
- If one or more supporting information for publication files have been uploaded, the manuscript file must have a "Supporting Information Available" paragraph just before the list of References.

Supporting Information for Publication

- Required data (such as images of NMR spectra or copies of crystallographic information files) must be included in the supporting information for publication.
- Images of NMR spectra must be combined into a single supporting information for publication file (or a small number of such files); they should not be uploaded as numerous separate image files.

Supporting Information for Review Only

- A copy of any published preliminary report, and any supplementary material associated with it, must be uploaded as a supporting information for review only file, and the report must be mentioned in the cover letter and cited in the manuscript.
- A copy of any cited "in-press" or "submitted-for-publication" paper must be provided as a supporting information for review only file.

Other

- Any previous submission of substantially the same manuscript to this or another ACS journal must be disclosed in the cover letter, and copies of the reviews appended to the cover letter. The cover letter should summarize the changes made in response to reviewer and editor comments.
- A Compound Characterization Checklist must be furnished if the manuscript reports the characterization of new or known compounds.

There are some additional less critical manuscript preparation and submission requirements that are listed in the Guidelines for Authors. Authors of manuscripts that qualify for priority processing will be asked to bring their manuscripts into compliance with these secondary requirements if the manuscript is accepted for publication. Authors of manuscripts requiring a pre-review revision will have the option of making these less important changes either during that revision, or after the review process if the manuscript is accepted.

COMPOUND CHARACTERIZATION CHECKLIST

JO _____ Page ____ of ____

Corresponding Author _____

Manuscript Title _____

1. Please copy this Checklist form and complete the form by hand.
2. Enter the name of the corresponding author and the title of the manuscript above. If this is a revised Checklist, enter the manuscript number next to "JO".
3. In the left-most column, enter the identifying numbers (or table-entry numbers) of the compounds or structures for which data are reported. List them in the sequence in which they appear in the experimental section (and in the supporting information, if there is any). For each compound, type a single "**X**" in either the "New" or the "Known" column.
4. For each compound or structure, place a single "**X**" in the columns corresponding to types of data reported in the experimental section and supporting information. You may use unlabeled columns for data types not listed. It is not expected that all or most of the columns be marked, only those needed to establish compound identity and purity.
5. Scan the completed Checklist, and save the scanned image(s) with file names that include the appropriate file extension (.pdf, .jpg, .gif), even on a non-Windows computer. Upload the saved file when submitting the manuscript. During file uploading, select "Compound Characterization Checklist" as the file designation.

COMPOUND			IDENTITY												PURITY					COMPUTATIONAL DATA in SI*		
Compound, structure, or table-entry number	New	Known	Melting point range	IR	UV-Vis	1H NMR	13C NMR	Other NMR [type: ____]	MS	HRMS	Optical rotation/ORD/CD	Enantiomeric/Diastereomeric ratio	X-ray [ORTEP and CIF in SI*]	Copy of 1H/13C NMR spectrum in SI*	Copy of chromatogram in SI*	Quant. GC, HPLC, or electrophoresis	Elemental analysis	Cartesian coordinates or Z-matrix	# of imaginary frequencies	Total energy	* SI = Supporting Information

CONTINUATION SHEET

JO _____ Page ____ of ____

COMPOUND CHARACTERIZATION CHECKLIST

Corresponding Author _____

COMPOUND			IDENTITY												PURITY					COMPUTATIONAL DATA in SI*		
Compound, structure, or table-entry number	New	Known	Melting point range	IR	UV-Vis	1H NMR	13C NMR	Other NMR [type:]	MS	HRMS	Optical rotation/ORD/CD	Enantiomeric/Diastereomeric ratio	X-ray [ORTEP and CIF in SI*]	Copy of 1H/13C NMR spectrum in SI*	Copy of chromatogram in SI*	Quant. GC, HPLC, or electrophoresis	Elemental analysis	Cartesian coordinates or Z-matrix	# of imaginary frequencies	Total energy	* SI = Supporting Information

AMERICAN CHEMICAL SOCIETY COPYRIGHT STATUS FORM

Please submit form to appropriate Editor's Office.

Name of ACS Publication:_____

Author(s):

_____
MS No.

Ms Title:

_____
Received

This manuscript will be considered with the understanding you have submitted it on an exclusive basis. You will be notified of a decision as soon as possible.

Print or Type Author's Name and Address

[THIS FORM MAY BE REPRODUCED]

COPYRIGHT TRANSFER

The undersigned, with the consent of all authors, hereby transfers, to the extent that there is copyright to be transferred, the exclusive copyright interest in the above cited manuscript, including the published version in any format (subsequently called the "work"), to the **American Chemical Society** subject to the following (If the manuscript is not accepted by ACS or withdrawn prior to acceptance by ACS, this transfer will be null and void.):

A. The undersigned author and all coauthors retain the right to revise, adapt, prepare derivative works, present orally, or distribute or transmit to not more than 50 colleagues, their own paper, provided that copyright credit is given to the source and ACS, that recipients are informed that they may not further disseminate or copy the paper, and that all such use is for the personal noncommercial benefit of the author(s) and is consistent with any prior contractual agreement between the undersigned and/or coauthors and their employer(s). Authors/employers may post the title of the paper, abstract (no other text), tables, and figures of their own papers on their own Web sites, and include these items in their own scholarly, research papers.

B. Where a work is prepared as a "work made for hire" for an employer, the employer(s) of the author(s) retain(s) the right to revise, adapt, prepare derivative works, publish, reprint, reproduce, and distribute the work in print format, and to transmit it on an internal, secure network for use by its employees only, and additional rights under A, provided that all such use is for the promotion of its business enterprise and does not imply endorsement by ACS.

C. Whenever the American Chemical Society is approached by third parties for individual permission to use, reprint, or republish specified articles (except for classroom use, library reserve, or to reprint in a collective work) the undersigned author's or employer's permission will also be required.

D. No proprietary right other than copyright is claimed by the American Chemical Society.

E. For works prepared under U.S. Government contract or by employees of a foreign government or its instrumentalities, the American Chemical Society recognizes that government's prior nonexclusive, royalty-free license to publish, translate, reproduce, use, or dispose of the published form of the work, or allow others to do so for noncommercial government purposes. Your contract number:_____

F. ACS reserves the right to use on the publication cover all figures submitted with the manuscript.

SIGN HERE FOR COPYRIGHT TRANSFER: I hereby certify that I am authorized to sign this document either in my own right or as an agent for my employer, and have made no changes to the current valid document supplied by ACS.

_____
Print Authorized Name(s) and Title(s)

☞ _____
Original Signature(s) (in Ink) Date

CERTIFICATION AS A WORK OF THE U.S. GOVERNMENT

I certify that **ALL** authors are or were bona fide officers or employees of the U.S. Government when the paper was prepared, and that the work is a "work of the U.S. Government" (prepared by an officer/employee of the U.S. Government as part of official duties), and, therefore, it is not subject to U.S. copyright. (This section should NOT be signed if the work was prepared under a government contract or coauthored by a non-U.S. Government employee.)

INDIVIDUAL AUTHOR **OR** AGENCY REPRESENTATIVE

Print Author's Name		Print Agency Representative's Name and Title
Original Signature of Author (in Ink)	Date	Original Signature of Agency Representative (in Ink)

☐ **WORKS SUBJECT TO CROWN COPYRIGHT:** If **ALL** authors are **bona fide** employees of the Governments of Australia, Canada, and the U.K., please check box and send to the appropriate Editor's Office for an alternative form (Blue Form). Control#0408317A