GUIDE FOR AUTHORS
(Revised January 2010)

Contents (Click on the topic)

The *Journal of Chemical Theory and Computation* invites new and original contributions with the understanding that, if accepted, they will not be published elsewhere. Papers reporting new theories, methodology, and/or important applications in quantum electronic structure, molecular dynamics, and statistical mechanics are appropriate for submission to this Journal. Specific topics include advances in or applications of ab initio quantum mechanics, density functional theory, design and properties of new materials, surface science, Monte Carlo simulations, solvation models, QM/MM calculations, biomolecular structure prediction, and molecular dynamics in the broadest sense including gas-phase dynamics, ab initio dynamics, biomolecular dynamics, and protein folding.

Manuscript Types

Articles

Full-length research manuscripts, consistent with the objectives of The *Journal of Chemical Theory and Computation*, are the principal focus of the Journal. Authors must follow the instructions for preparation and submission given below.

Perspectives

Perspectives are interpretive accounts on subjects of current interest to the JCTC community. This series is intended to be a forum for experts to present their perspectives on emerging or active areas of research.

Letters

Letters are intended for rapid publication of preliminary reports on important findings of novel and timely significance. The major concepts of the paper should not have been published previously. Manuscripts are limited to four journal pages (16 double-spaced manuscript pages including all materials). The abstract is limited to 75 words and should briefly state the purpose of the research, principal results, and major conclusions.

Supporting Information can be provided detailing procedures and providing supplementary data.

Manuscripts must be submitted electronically via the secure Web site at http://pubs.acs.org/page/4authors/submission/index.html. Guidelines for this method are provided here. If substantially the same manuscript has been previously submitted to this Journal or to another ACS journal, the author should include copies of the reviews with the submission and explain any revisions in the cover letter. The Editor may accept the manuscript on the basis of those reviews and author remarks or may seek additional reviews.

For further inquiries contact the Editor-in-Chief, Prof. William L. Jorgensen, Department of Chemistry, Yale University, P.O. Box 208107, New Haven, CT 06520-8107. Phone: 203-432-4118. Fax: 202-513-8628. E-mail: eic@jctc.acs.org.

Preparation of Manuscript

Submission

A guide to the proper format for manuscripts is provided on the Journal's Web page, on http://pubs.acs.org. Another valuable resource is *The ACS Style Guide*, 3rd ed. (2006) available from Oxford University Press, Order Department, 201 Evans Rd, Cary, NC 27513. This book deals with all questions relating to manuscript style and provides the standard list of abbreviations for ACS Journals.

Authors must be sure that they are familiar with and abide by the Ethical Guidelines that are also available on the Web site and in *The ACS Style Guide*.

The title of the paper should be brief-preferably 12 words or fewer. Readers rarely read and absorb longer titles, so it should be concise. An abstract of 3-4 sentences is required, and as with the title, it should be concise, touching on just the major points about which the author wants to alert the reader.

References in the text should be identified with superscript numbers (e.g., Jones[14] has shown...). In the Web edition of the Journal, each reference has a "CAS" tag that can be used by readers to retrieve the corresponding CAS abstract, and for this to be successful, accuracy in the reference is critical. References may or may not contain the title but must contain the starting and ending pages of the paper cited, thus

> (8) Sustmann, R.; Sicking, W.; Huisgen, R. A Computational Study of the Cycloaddition of Thiobenzophenone S-Methylide to Thiobenzophenone. *J. Am. Chem. Soc.* **2003**, *125*, 14425-14434.

References to books should cite the author(s), title, publisher, publication date, and page(s). In referring to a book written by various contributors, the author(s) should be cited first, as in

> (8) Weinstein, S.; Henderson, R. B. In Heterocyclic Compounds; Elderfield, R. C., Ed.; Wiley: New York, 1950; Vol. 1, Chapter 1, pp 60-65.

Authors are encouraged to use Supporting Information (SI) in cases where manuscripts contain extensive tables of data or source codes that are of interest to particular readers. The pages of SI should be numbered sequentially, should be labeled as SI, and should be readily legible. The production staff will not alter the appearance of Supporting Information. A paragraph that briefly describes the Supporting Information, providing only the information necessary to access the

data, should be included and should be terminated as follows: This material is available free of charge via the Internet at http://pubs.acs.org.

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Submission of Manuscript

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Revision of Manuscript

Submission

When reviews of the paper have been completed, they will be sent to the author electronically by e-mail. The manuscript should be revised so as to address each one of the comments made by the reviewers. Then the manuscript should be resubmitted through the Web site following the steps for submitting a revised manuscript. A letter describing the responses made by the author to each of the comments from the reviewers should also be sent. This letter is required and can be submitted over the Web along with the revised manuscript. **A Copyright Status form is also required; the paper will not be processed further until both these documents are received.** The copyright form can be obtained from http://pubs.acs.org/copyright.

Publication of Manuscript

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Editorial Production

Text

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The article should conform to the usual ACS format, which is described at pubs.acs.org. The final version should be prepared in a single word-processor file, with all graphics included.

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The fonts "Times" and "Symbol" produce the best results. Other fonts, particularly those that do not come bundled with the system software, may not translate properly. All special characters (e.g., Greek characters, math symbols, etc.) must be present in the body of the text as characters and not as graphic representations.

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The quality of the graphics in the Journal depends on the quality of the originals provided by the author. Figures cannot be modified or enhanced by the Journal production staff. Whenever possible, the graphics files furnished by authors with Web submissions are used in production of the Journal. The following guidelines may be helpful.

Unless dealing with a color graphic, figures and diagrams should be totally black and white. Graphics should be inserted into the electronic manuscript at the appropriate place. Illustrations should be submitted in the actual size that is desired in the final publication and should fit either a single-column (maximum 8.25 × 24 cm) or a double-column (10.5-17.78 × 24 cm) format. Text in the graphics should be no smaller than 4.5 pts.

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(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%

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Nomenclature

It is the responsibility of the authors to provide correct nomenclature. Nomenclature should conform with current American usage. Insofar as possible, authors should use systematic names,

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