

# *Journal of Computer Chemistry, Japan -International Edition*

## **Information for Authors, 2016**

### 1. Submission of Manuscripts

#### 1.1 Manuscripts and Articles

##### 1.1.1 Manuscripts

The *Journal of Computer Chemistry, Japan -International Edition* (JCCJIE) will publish the following kinds of contributions.

**General Papers:** Complete reports of original work on computational methods, hardware and/or software for chemical research or chemical theory or development or applications in the broadest sense.

**Notes:** Brief reports of novel developments or applications (maximum length : 4 journal pages).

**Technical Papers:** Reports of technically original work, for example, the implementation of a program for wider applicability.

**Reviews:** Creative reviews on timely topics in areas appropriate to the Journal.

**Accounts:** Concise and objective reviews, the contents of which are largely from the author's own laboratory.

**Letters:** Selected Papers from the Annual Spring (Autumn) Meeting.

##### 1.1.2 Articles

**Commentary:** Expressions of opinions or explanations about computer chemistry. It should be written in an accessible, non-technical style and does not normally contain primary research data, although it may present 'sociological' data.

**Highlights:** Brief descriptions of outstanding part of a notable study in computer chemistry.

**Software News and Reviews:** Reviews of computer applications software. It may be accepted when written by application dealers. No page charge will be requested when the author puts an advertisement in the journal.

### 1.2 Electronic Submission Instructions

All manuscripts should be submitted using the *Journal of Computer Chemistry, Japan* (JCCJ) web-based manuscript submission and handling system at the URL below.

**ScholarOne Manuscripts Online Submission System** for JCCJ.

[ScholarOne Manuscripts](http://mc.manuscriptcentral.com/jccj) (<http://mc.manuscriptcentral.com/jccj>)

The following electronic files should be prepared for each electronic submission:

- **Main Document** file (MS-Word recommended) containing title page, abstract, text, references, figure legends, and table captions.
  - Figures and/or tables (**Illustration** and **Table** files).
  - Supplementary material (**Supplementary Files**).
- (See Appendix 1 for available files).

**ScholarOne Manuscripts** will automatically convert these uploaded files into single PDF and HTML documents so that they can be viewed and printed for peer reviewing. Authors must verify that the PDF and HTML files are satisfactory and complete.

Authors should enter the supporting information the follows:

Information about manuscript (issue type, kind of paper), Title, Information about authors

(Corresponding author's name, full mailing address, telephone number, facsimile number and e-mail

address), Membership No. (One of the authors must be a member of SCCJ).

#### 1.2.1 Submitting Process:

You will follow the submission steps:

- (1) Enter manuscript information such as title etc.
- (2) Upload manuscript file(s).
- (3) Edit your input if necessary.
- (4) Confirm your input.

When the information for your submission is saved, a manuscript number is automatically generated.

Using your ID and a Password, you can log onto your page at any time.

After you have received e-mail for corrections, you must resubmit via the Website within two weeks.

Each revised manuscript must be accompanied by a covering letter that addresses each of the comments of reviewer (s) and explains all changes made in the earlier version.

#### 1.3 Hardcopy Submission Instructions

Authors are encouraged to submit using the *Journal of Computer Chemistry, Japan (JCCJ)* web-based manuscript submission and handling system **ScholarOne Manuscripts**. However, conventional, hardcopy submissions are also acceptable.

Postal address:

Tatsuya Tachikawa (Ph. D.), JCCJ Editorial Office,

Course of Applied Chemistry, Programs in Chemistry, Graduate School of Science and Engineering,  
Saitama University,

255 Shimo-Ohkubo, Sakura-ku, Saitama, Saitama, 338-8570 JAPAN

Please contact us if you have any questions. e-mail: [jccjoffice@sccj.net](mailto:jccjoffice@sccj.net)

#### 1.4 Publication

After proofreading, each manuscript that is accepted for publication will be published electronically through the Internet prior to the conventional publication in printed form. All the articles appearing in *Journal of Computer Chemistry, Japan* are to be made available through international network WWW (World Wide Web). In case of problems, the *Society of Computer Chemistry, Japan* has no responsibility to continue this service.

Members of *Society of Computer Chemistry, Japan* may share their subscriptions in conventional printed form without further cost. Member and subscription services are available from the following.

Society of Computer Chemistry, Japan

2-1-13-607 Higashiueno, Taito-ku, Tokyo 110-0015 JAPAN

TEL080-2388-0894 ; FAX 03-5830-3922 ; e-mail : [sccjoffice@sccj.net](mailto:sccjoffice@sccj.net)

URL: <http://www.sccj.net>

#### 1.5 Page Charges

To defray some of the cost of conventional publication, a payment (shown in Table 1) is required. On payment of the page fee, authors receive CD-R without further charge.

Table 1. Page Charge / in Japanese Yen

pages	1–2	3–4	5–6	7–8	9–10	over 10 pages
Charge for Member	20,000	30,000	40,000	50,000	60,000	10,000 per 2 pages
Charge for Nonmember	25,000	35,000	45,000	55,000	65,000	10,000 per 2 pages

## 1.6 Copyright

The JCCJ Copyright Transfer Form (JCCJ CTF) is found at the end of this section. The Editorial Office will send the JCCJ CTF to principal author before advanced publication. The JCCJ CTF must be completed and signed for each submitted manuscript. No substitute forms or attachments are acceptable. The signed form have to be sent to the Editor assigned to the manuscript by mail, facsimile or attached scanned file with e-mail.

**Postal address:** Tatsuya Tachikawa (Ph. D.), JCCJ Editorial Office,  
Course of Applied Chemistry, Programs in Chemistry, Graduate School of Science and Engineering,  
Saitama University, 255 Shimo-Ohkubo, Sakura-ku, Saitama, 338-8570 JAPAN

**facimile:** +81-48-858-9274

**e-mail:** jccjoffice@sccj.net

No paper is released for publication until an author's corrected proof has been returned. The copyright of papers accepted for publication in *Journal of Computer Chemistry, Japan* belongs to the *Society of Computer Chemistry, Japan* (SCCJ). The transfer of copyright from author to the Society must be explicitly made to enable the Society to ensure maximum dissemination of the author's work.

The author(s) may, without seeking permission from JCCJ, make available the PDF (Portable Document Format by Adobe Systems Inc.) of the paper via personal website(s) of the author(s) or via the Internet of the organization(s) where the author(s) work(s) providing that the following statement appears on the first page, or screen, of the Paper as posted on the server:

Copyright 200x Society of Computer Chemistry, Japan. : The right header of the first page.

DOI: 10.2477/jccj.Hxxxx : The left footers of all odd pages.

## 2. Preparation of Manuscripts

We have not prepared a template for Electronic Submission. Please write your manuscript in accordance with this guideline.

### 2.1 General Instructions

- The entire manuscript must be submitted on good quality A4 (21.0 x 29.6 cm) paper with 3.0 cm top and bottom margins, if submitted as Hardcopy.
- The title should have a column width of 15 cm (margins of 3.0 cm on the right and left sides) with a character size of 16 points in Times bold. The title of the article should be centered, in capitals for the first letter of each word except for articles, conjunctions, and prepositions. The names of the authors (12 points) and addresses (9 points) at which the research was done should appear under the title and have a column width of 15 cm in a Times font. Use the letters a, b, c..., as superscripts to link authors to their addresses and an asterisk to indicate the author(s) to whom correspondence should be addressed. Complete addresses should be given, including postal zip

codes. The e-mail address of the author to whom correspondence should be addressed should be given in italics.

- (c) The date received is the day on which the editor receives the article. The Editorial Office enters the date received after the addresses.
- (d) The abstract (column width of 16 cm (margins of 2.5 cm on the right and left sides)) and text (column width of 17 cm (margins of 2.0 cm on the right and left sides)) must have single spacing, full justification, and a character size of 9 points. A Times font is recommended. Superscript and subscript letters or numbers must be at least 2.2 mm high. Indent the first sentence several spaces. The abstract should be written so that readers can understand the purpose, methods and conclusions without referring to the text. Do not use a heading in the abstract. When a compound, Table or Figure number is cited in the abstract, such numbers should be identical with those used in the text. After writing several keywords (for example, Keywords : Crystal structure, Molecular orbital, Curve fitting, Multimedia, Chemical education), begin the text. The first sentence is written in two-step sets, after the title, names, affiliations, abstract, keywords of the head. Use headings for Introduction, Method (instruments, operation system, etc.), Experimental Part, Results and Discussion, Conclusion, etc. Expressions of thanks should be brief and placed before the References and Notes section, but with no heading. All pages should be numbered consecutively.
- (e) The references to the literature and footnotes (except those in Tables) should be numbered in the text in one consecutive series. For example: Hosoya *et al.* [1, 2] by Yoshimura [3 - 6], Newbold [7], and Yoshino [8]. The list of literature cited and footnotes should be headed by the phrase References and Notes and numbered 1, 2, 3, *etc.*, according to the numbers used in the text. Journals should be abbreviated as in Chemical Abstracts. The use of "ibid." and "idem" in references is not allowed. In references, the journal title and the volume number (or year, if there is no volume number) should be typed in italics and bold-face, respectively. If reference is made to a paper submitted for publication or in press, authors are required to enclose a copy of the manuscript or galley proof.
- (f) A statement of the availability or the manner of distribution of each program appearing in the text is required.
- (g) The title in English, authors and their affiliations, telephone and facsimile numbers, e-mail address of the principal author and abstract in English are to be placed at the end of each manuscript written in Japanese.

## 2.2 Nomenclature, Symbols, Units, and Abbreviations

Nomenclature should conform as closely as possible to the rules established by IUPAC. Symbols and units should conform as closely as possible to SI units. The preferred forms for a few of the commonly used abbreviations and units are mp, bp, s, min, h, g, mg, m, cm, nm, Hz, ppm, MOPAC, AM1, PM3, TLC, NMR, UV, and IR.

[SI Units: Bureau International des Poids Mesures (BIPM)]: <http://www.bipm.org/en/si/>

[A conversion tables from non SI to SI]:

[http://www.bipm.org/en/si/si\\_brochure/chapter4/table6.html](http://www.bipm.org/en/si/si_brochure/chapter4/table6.html)

## 2.3 Tables and Figures

- (a) Tables and Figures must have a width of 17 cm (full column) whenever possible. The citations of figures should be made in accordance with the following examples: Figure 1; Figures 1, 2, and 3. "Figure" should be spelled out instead of being written "Fig." For Tables and Figure captions, a

Times font with a character size of 9 points is recommended. Standard abbreviations should be used in Tables. For "Table" in headings and "Figure" in captions, a Times bold font is recommended: for example: Table 2.; Figure 1. Footnotes in Tables are indicated by the letters a, b, c, etc. as superscripts and without parentheses. For footnotes in Tables and Figure captions, a character size of 9 points and single spacing may be used. Mathematical and chemical equations should be arranged to occupy a single column. Authors using computer graphics and desktop-publishing software are encouraged to incorporate Formulas and Schemes in the text (one column) where they are to appear.

- (b) Structural or displayed formulas must be accurately drawn or typed. The illustrations should be clear enough for photographic reproduction. Color illustrations are acceptable providing that their black-and-white images give sufficient information. They will be published electronically in color; however, in the form of conventional printing, they will be published only in black-and-white.

#### 2.4 Supplementary material

Supplementary material may be submitted for online-only publication if it adds value for potential readers. However, it must not contain material critical to the understanding of the manuscript. The hard copy of the manuscript should stand alone, but it should be indicated at an appropriate point in the text that supplementary material is available online. In addition, the availability of supplementary material should also be indicated in the manuscript by a section headed 'Supplementary material' with a brief description of these data to appear before the Acknowledgements and References. If possible, the best format to present these data is a single PDF file. Please include the manuscript title and list of authors on the first page, and whenever possible include the figure legends. Supplementary material should be named and cited within the manuscript as Figure S1, Table S1, Video S1, etc. Supplementary material is available to reviewers and editors during the review process. If images are supplied as .GIFs or .JPEGs, the minimum acceptable resolution for viewing on screen is 120 dpi.

#### 2.5 Graphical Abstract

When you upload the final manuscript, please add a Figure to the end of main document for a "Graphical Abstract". The Graphical Abstract is a visual summary of the main findings of the article. This could either be the concluding figure from the article or a figure that is specially designed for the purpose.

## ScholarOne Manuscripts Files Available for uploading

	◎ : ScholarOne Manuscripts will automatically convert these uploaded files into single PDF and HTML.	
Kind of file/extension	Japanese	English
Word (doc)	◎	◎
Word (docx)	◎	◎
pdf	◎	◎
rtf	◎	◎
odt	○	○
txt	△	◎
LaTeX (Using Template) (Avoid macros)	○	○
tif	◎	◎
gif	◎	◎
jpg	◎	◎
eps	◎	◎
psd	◎	◎
png	◎	◎
Postscript	◎	◎
PICT	◎	◎
Excel (xls)	◎	◎
Excel (xlsx)	◎	◎
PowerPoint (ppt)	◎	◎
The others	Image: bmp, ai etc. Animation: OK	

*Journal of Computer Chemistry, Japan* Submission / Copyright Transfer Form

Manuscript No. :

Authors' Names, Affiliations and Addresses

Corresponded author's e-mail address

Dates received and accepted

I / We submit to *Journal of Computer Chemistry, Japan* the manuscript specified below. I / We certify that the work reported here has not received prior publication and is not under consideration for publication elsewhere in any medium.

Type of Paper/ Article: General Paper \_\_\_\_\_, Note \_\_\_\_\_, Technical Paper \_\_\_\_\_, Review \_\_\_\_\_, Account\_ Commentary \_\_\_\_\_, Highlights \_\_\_\_\_, Software News and Reviews \_\_\_\_\_, Letter \_\_\_\_\_

Number of manuscript pages: \_\_\_\_\_, Page charge: \_\_\_\_\_ (Japanese Yen)

Original Source Program File: Enclosed \_\_\_\_\_ Not enclosed \_\_\_\_\_

Do you want to distribute any programs appearing in the manuscript by way of the *Society of Computer Chemistry, Japan* (SCCJ)? Yes \_\_\_\_\_ No \_\_\_\_\_

\*\*\*\*\*COPYRIGHT TRANSFER\*\*\*\*\*

I / We agree to transfer to *Society of Computer Chemistry, Japan* (SCCJ) the copyright of the above-mentioned manuscript, when the manuscript is accepted for publication in The Journal in any form.

Author's signature \_\_\_\_\_ Date \_\_\_\_\_

The author(s) may, without seeking permission from JCCJ, make available the PDF (Portable document format from Adobe Systems Inc.) of the Paper via personal website(s) of the Author(s) or via the Internet of the organization(s) where the Author(s) work(s) providing that the following statement appears on the first page, or screen, of the Paper as posted on the server:

Copyright 200x Society of Computer Chemistry, Japan. : The right header of the first page.

DOI: 10.2477/jccj.H\*\*\*\* (manuscript No.) : The left footers of all odd pages.

This paper was published in "x. xxxx, x. xxxx and x. xxxxx (author's name (s)), *J. Comput. Chem. Jpan.*, xx (Vol. No.), xxx-xxx (pages), xxxx (year). The internet address of the above Journal is as follows:

[http://www.sccj.net/publications/JCCJ/v5\(Vol. No.\)/n3\(issue No.\)/a12\(article No.\)/document.pdf](http://www.sccj.net/publications/JCCJ/v5(Vol. No.)/n3(issue No.)/a12(article No.)/document.pdf)