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3 Editorial procedure

TCA considers for publication, in English language, three kinds of manuscripts: **overviews**, **regular articles** and **letters**. All papers should be of interest to researchers in the areas of chemical theory, computation, and modeling. All branches of chemistry (e.g., physical, organic, inorganic, polymer, biological, materials, etc.) are included.

Overviews should summarize recent progress in a specific field and should be written in a style that addresses the broad theoretical and computational chemistry community. Accounts are normally restricted to 24 double spaced typed pages (in 12 point font), including tables and references. In addition, up to eight figures may be submitted.

Regular articles should report work of particular interest to specialists in the theoretical and computational chemistry fields. Examples of such work include numerical methods, new developments in analytical theory, parameterization and force field validation, basis set developments, new algorithms and testing of prototype applications that are noteworthy for breaking new ground or illustrating the capabilities of methods, and so forth. There is no restriction on manuscript size; brevity is encouraged insofar as scientific content allows.

Letters are normally restricted to 12 double spaced typed pages (in 12 point font), including tables and references. In addition, up to six figures may be submitted.

TCA invites submission of reports from symposia, workshops, and conferences of interest to our readers for publication in either the printed version of the journal or the internet archive. Such reports should contain results of interest to theoretical and computational chemists or modelers. Reports which provide a snapshot of the status of some subfield or research topic are most welcome; and those consisting mainly of lecture titles without results or conclusions are not appropriate for publication in TCA.

In lieu of electronic submission 3 copies of the manuscript should be sent to an advisory editor who is familiar with the research area. Submissions may also be sent to the editor or associate editor, in which case a list of six or more potential referees should be provided. Review within four weeks of receipt is guaranteed for Letters, while other submissions will be handled with all due alacrity.

Please be sure to include your e-mail address and your fax number.

The manuscripts and the figures will not normally be returned, unless specifically requested by the authors.

4 Manuscript preparation

Manuscripts should be typed in double-line spacing throughout on one side of the paper only and with at least 2.5 cm (1 inch) margins.

When initially submitted electronically, the entire manuscript including all figures, tables, schemes or structures, should be transmitted as a single .pdf file. Original electronic files are not required prior to the end of the review process.

To help you prepare your manuscript, Springer offers a template that can be used with Winword 7 (Windows 95), 97, 2000, and Word for Macintosh. For details see point 4.

For authors who prepare their papers in LaTeX Springer offers the macropackage LaTeX2e document class `svjour2` (see Sect. 5).

Authors who wish to submit disks to the editor **must include any macro definitions** they have used together with a printout for reference. It is important to ensure that the text is identical in the hard copy and in the soft copy.

The production time for papers submitted in this form can be reduced considerably. Authors who have written their papers in TeX but have not used Springer's macros should likewise send in a disk and corresponding hard copy. Springer will then decide on a case-by-case basis whether it makes sense economically to work from the TeX files.

All manuscripts are subject to copy editing.

■ Title page

- A concise and informative title
- The name(s) of the author(s)
- The affiliation(s) and address(es) of the author(s)
- The e-mail address, telephone and fax numbers of the communicating author

■ **Abstract.** Each paper must be preceded by an abstract presenting the most important results and conclusions in no more than 150 words

■ **Keywords.** 3 to 6 keywords taken from Chemical Abstract or other sources should be supplied after the Abstract for indexing purposes.

■ **Footnotes** on the title page are not given reference symbols. Footnotes to the text are numbered consecutively; those to tables should be indicated by superscript lower-case letters (or asterisks for significance values and other statistical data).

■ **Chemical formulae and names** as well as the names of organisms must be unambiguous and in accordance with the relevant international recommendations, cf. "IUPAC (1993) Quantities, Units and Symbols Trade, Blackwell Scientific, Oxford" and "ISO (1993) International Vocabulary of Basic and General Terms in Metrology", Geneva. Trade names should be avoided; abbreviations and uncommon symbols should be explained at first mention.

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■ The **Introduction** should state the purpose of the investigation and give a short review of the pertinent literature.

■ The **Materials and methods** section should follow the Introduction and should provide enough information to permit repetition of the experimental work.

■ The **Results** section should describe the outcome of the study. Data should be presented as concisely as possible, if appropriate in the form of tables or figures, although very large tables should be avoided.

■ **Acknowledgements.** These should be as brief as possible. Any grant that requires acknowledgement should be mentioned. The names of funding organizations should be written in full.

■ **Appendix.** If there is more than one appendix, they should be numbered consecutively. Equations in appendices should be designated differently from those in the main body of the paper, e.g. (A1), (A2) etc. In each appendix equations should be numbered separately.

■ The list of **References** should only include works that are cited in the text and that have been published or accepted for publication.

Citations in the text should be identified by *numbers in square brackets*, and the list of references at the end of the paper should be numbered.

Book titles are given, but titles of journal articles are not.

Here are a few examples for the style of references:

Journal
Grissom LE, Harcke HT (1997) *Pediatr Radiol* 27: 70-74

Books
Larcher W (1995) *Physiological plant ecology*, 3rd edn. Springer, Berlin Heidelberg New York

Inzelt G (1994) Mechanism of charge transport in polymer-modified electrodes. In: Bard AJ (ed)

Theoretical Chemistry Accounts

Theory,
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Instructions for Authors, continuation

Electroanalytical chemistry, vol 18. Dekker, New York Basel Hong Kong, pp 89–241

If available the **Digital Object Identifier (DOI)** of the cited literature should be added at the end of the reference in question.

Example: Ward J, Robinson PJ (2002) How to detect hepatocellular carcinoma in cirrhosis. *Eur Radiol* 12:2258-2272. DOI 10.1007/s00330-002-1450-y

References such as “personal communications” or “unpublished data” cannot be included in the reference list, but should be mentioned in the text in parentheses; this also applies to papers presented at meetings but not yet published or accepted for publication. A date should be given for both “personal communications” and “unpublished data”.

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Line drawings. Please submit good-quality prints. The inscriptions should be clearly legible.

Half-tone illustrations (black and white and color). Please submit well-contrasted photographic prints with the top indicated on the back. *Magnification* should be indicated by *scale bars*.

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For all categories of manuscripts, **colour figures** will be published free of charge when warranted by content.

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Please send only the final version of the article, as accepted by the editors.

Preparing your manuscript

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LaTeX:

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1. Use a normal, plain font (e.g., Times Roman) for text.

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Data formats

Save your file in two formats:

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- On a ZIP cartridge
- On a CD-ROM

Please always supply the following information with your data: journal title, operating system, word processing program, drawing program, image processing program, compression program.

6 Electronic supplementary material

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After acceptance by the journals Editor(s) ESM will be published as received from the author in the online version only. Reference will be given in the printed version.

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