

HELVETICA CHIMICA ACTA

Instructions for Authors (2004)

1. General Policy

The journal *Helvetica Chimica Acta* (*HCA*) invites selected original and significant contributions of fundamental research in all branches of the theory and practice of chemistry. The critical selection criteria are originality and quality of the work, as well as the breadth of interest to readers and subscribers.

Contributions are considered from non-members as well as members of the *Swiss Chemical Society*. Manuscripts may be submitted for publication as *Articles*, *Notes*, and *Preliminary Communications*; *Review Articles* are only occasionally accepted for publication in *HCA*.

Contents of manuscripts submitted to *HCA* must not have been published previously, except in the form of a brief preliminary communication, nor have been submitted to another journal.

Manuscripts should be submitted in *triplicate*, together with the *electronic version* and a transmittal letter signed by the author to whom correspondence should be addressed, to:

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Receipt of a manuscript for consideration will be acknowledged by the Editorial Office *via* mail¹⁾. This acknowledgement will indicate the *manuscript reference number*, which must be quoted in all subsequent correspondence. (A manuscript requiring substantial revision prior to publication that is not returned to the Editorial Office within *two months* will be treated as a new submission, *i.e.*, will be assigned a new reference number.)

Submission of a manuscript implies that the authors agree to transfer copyright to the *Verlag Helvetica Chimica Acta AG* when the contribution is accepted for publication. Reproduction of the text, figures, or tables from *HCA* is allowed only with permission of the Editorial Office.

¹⁾ When an e-mail address is available, the receipt will be acknowledged by e-mail.

2. Preparation of Manuscripts

2.1. General Considerations. Careful preparation of the manuscript and adherence to the format and conventions of *HCA* as laid down in these *Instructions for Authors* will facilitate rapid publication. Authors should consult recent issues of *HCA* for examples.

Manuscripts may be submitted in English, German, French or Italian. Manuscripts must be prepared with a word processor (preferred) or typewriter and be printed *double-spaced* to allow for editorial markings. Authors are requested to reserve margins of at least 3 cm at the top and bottom of each page and at least 4 cm on the left-hand side. Copies made by a clearly legible duplication process are preferred. Computer-processed manuscripts produced by a matrix printer of low quality are undesirable.

Pages should be numbered consecutively beginning with the title page. References, tables, scheme and/or figure legends, formula collections, schemes, and figures **must** be grouped together **in this order** at the end of the manuscript and numbered accordingly. Original drawings of formulae, schemes, and figures should be furnished together with the manuscript.

A representative structural formula or scheme should be provided for the Table of Contents. The maximum available place for this graphical abstract is 3 × 10 cm.

Authors who are not fully fluent in English are strongly advised to seek assistance from a fluent colleague when preparing a manuscript. In all cases, it is wise to consult a standard manual of style (e.g., 'The ACS Style Guide: A Manual for Authors and Editors', Ed. J. S. Dodd, 2nd edn., American Chemical Society, Washington DC, 1997, or W. Strunk Jr., E. B. White, 'The Elements of Style', 4th edn., Prentice Hall, New York, 1999 (also found at <http://www.bartleby.com/141/index.html>)). Manuscripts containing grammatical and/or stylistic deficiencies are handicapped during the review and editorial processes, leading to *rejection* or *significantly longer publication times*.

Manuscripts should be kept to minimum length, and for clarity, each work should be subdivided into labeled sections, e.g., **Introduction, Results, Discussion, Experimental Part**.

Special types of print should be indicated as outlined in the Table.

Table. *Specification of Typeface*

Type	Mark	Symbol	Example	Example (printed)
Boldface ^{a)}	Single underline	<u> </u>	Introduction	Introduction
Italic ^{b)}	Wavy underline	<u>~~~~~</u>	<i>in vitro</i>	<i>in vitro</i>
Small capital ^{c)}	Double underline	<u>=====</u>	0.5M	0.5M
Boldface italic ^{d)}	Underline with wavy line	<u>~~~~~</u>	<i>R</i>	<i>R</i>

^{a)} Headings, designated numbers of chemical compounds.

^{b)} Subheadings, configurational prefixes ((*R*)-, (*S*)-, *cis*-, *trans*-, etc.), Latin words or abbreviations, trade names of chemical compounds (first letter should be capitalized), names of authors if mentioned in the text.

^{c)} Symbols of molar and normal concentrations (M and N), D and L, the names of the nomenclature of genera, species, or varieties.

^{d)} The italicized terms and prefixes in headings.

Special characters not available on a typewriter should be clearly drawn in ink and explained unambiguously in the margin on first appearance.

2.2. Title Page. For the layout of the title page, a current issue of *HCA* should be consulted.

Attention is drawn to the following points:

a) The title of a manuscript, being of greatest importance for current awareness and information retrieval, should clearly and accurately provide information on the content and emphasis of the work. The use of abbreviations, symbols, chemical formulae, and references in a title is strongly discouraged. First letters of nouns and adjectives are capitalized.

b) The authors' full first names, middle initials, and last names should be given, followed by the address(es) of the contributing laboratory or laboratories. The author to whom correspondence and/or inquiries should be directed should be indicated by an asterisk (*). Footnotes may be added to indicate the present mailing address(es) of the author(s). The corresponding author's mailing address, phone number, fax number, and e-mail address should also be included.

2.3. Abstract. The second page of the manuscript should be reserved for an abstract in English, independent of the language of the main text. If this is German, French, or Italian, the abstract should be preceded by an English translation of the title. ***The abstract, stating briefly the purpose of the research (if not clear from the title), the principal results, and major conclusions, should be self-explanatory and intelligible without reference to the text.*** References to structural formulae, *Tables*, *Schemes*, and *Figures*, by number, may be made in the abstract. For a typical contribution, an 80- to 200-word abstract is usually adequate.

2.4. References. References should be numbered sequentially in the order they are cited in the text. The numbers should be set in brackets, thus [2] or [3] [14]. References, typed with double spacing, are to be collected in numerical order at the end of the main text. Titles of journals must be abbreviated according to *Chemical Abstracts* (cf. *Chemical Abstracts Service Source Index (CASSI)* and *Appendix I*).

Attention is drawn to the following conventions: a) Names of all authors of cited publications should be given. Use of 'et al.' in the list of references is not accepted. b) Only the initials of first and middle names should be given. c) The name of the journal and volume number cited should be given in italics [1]. d) Composite references may be used, instead of a series of individual ones [2]. The use of the Latin terms *ibid.* and *idem* is no longer allowed, since these are not compatible with electronic information-retrieval systems [3]. When a part of a composite reference is cited individually in the text, the parts of the composite reference may be specified by a), b), etc. [4a][4b]. e) In references described as 'personal communications', an affiliation should follow the name(s) of the person(s) cited [5]. f) Descriptions such as 'for a review, see . . .' should be included in the body of the text and not as part of the reference.

Examples of references to book chapters [6], books [7], patents [8], computer programs [9], and Ph.D. theses [10] are also given.

REFERENCES

- [1] M. Barbero, I. Degani, S. Dughera, R. Fochi, L. Piscopo, *J. Chem. Soc., Perkins Trans. I* **1996**, 289.
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- [4] a) J.-P. Bourgeois, F. Diederich, E. Echegoyen, J.-F. Nierengarten, *Helv. Chim. Acta* **1998**, 81, 1835; b) E. Dietel, A. Hirsch, E. Eichhorn, A. Rieker, S. Hackbarth, B. Röder, *Chem. Commun.* **1998**, 1981.
- [5] H. Vančik, (Faculty of Natural Sciences, University of Zagreb), personal communication.
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- [7] J. D. Dunitz, 'X-Ray Analysis and the Structure of Organic Molecules', Verlag Helvetica Chimica Acta, Basel, and VCH, Weinheim, 1995.
- [8] T. Kamata, N. Wasada, Jap. Pat. 2-204469, 1990, p. 381–384.
- [9] G. M. Sheldrick, SHELXL97, Program for the Refinement of Crystal Structures, University of Göttingen, Germany, 1997.
- [10] B. R. Peterson, Ph.D. Thesis, University of California at Los Angeles, 1994.

In the text, reference to author(s) of cited works should be made without giving initials, e.g., '...as shown by Kamata and Wasada [8]'. If the reference carries the names of three or more authors it should be quoted as 'Barbero *et al.* [1]', if Barbero is the first author, or as 'Piscopo and co-workers [1]', if Piscopo is the senior author.

2.5. Footnotes. Footnotes, *i.e.*, explanations or comments on the text, should be kept to a minimum. Each one should be indicated in the manuscript by a superscripted number followed by a closing parenthesis, e.g., '...is implied¹⁾', otherwise...', and numbered sequentially throughout the manuscript. Each footnote should be typed **double-spaced** at the bottom of the page of the manuscript in which it is first mentioned. Footnotes must not be included with the references.

2.6. Tables. Tables should be used only where the information is more effectively presented in tabular form than in the body of the text. Each table must be referred to in the text, given suitable captions, typed on separate sheets, and placed after the references. Column headings should be as short as possible but must define units unambiguously. When necessary, an abbreviated or symbolic column heading should be used and explained in the table-heading or in a footnote. Footnotes to tables should be labeled ^{a)}, ^{b)}, ^{c)}, *etc.*, and typed at the bottom of the table. Tables should be prepared to fit the page format of *HCA*.

2.7. Structural Formulae, Schemes, and Figures. Laser prints, line drawings, or sharp glossy photographs (no Xerox or similar copies) of the figures and structural formulae should be submitted with the manuscript. Copies must be included with each copy of the manuscript. Original drawings of standard size A4 are preferred, and they must contain all necessary symbols and lettering, *i.e.*, they must be usable without additional artwork by the *HCA* printers.

Line thickness, line spacing, and, especially, the size of all the necessary symbols and lettering should be planned for optimal legibility after photoreduction to 12.5-cm width. All atom labels and text should be in 'plain' style (lightface), and compound numbers should be in boldface type. Computer-plotted drawings must satisfy the same criteria.

Original drawings or photographs should be identified with the author's name and numbered to agree with the figure legends.

Structural formulae will not be type-set and must, therefore, be provided by the authors ready for reproduction. They should be combined in suitable schemes to reduce the cost of block-cutting. In general, only displayed formulae should be given boldface key numbers; compounds mentioned only in the text should be referred to by name.

For authors using the *ChemDraw* program, the following procedure is recommended.

1. The following 'preferences' should be selected: bond spacing 14% of width, 10-pt *Helvetica* font for atom labels, 12-pt *Helvetica* font for captions, fixed length 17 pt (0.6 cm), bold width 2.9 pt (0.101 cm), line width 0.54 pt (0.019 cm), margin width 2.0 pt (0.071 cm), hash spacing 2.0 pt (0.071 cm).
2. The page setup should be set to 100%.
3. With the *ChemDraw* ruler or appropriate margin settings, a maximum width of 16.8 cm should be created for structure blocks, schemes, and equations.
4. Compound numbers should be in boldface type, but not atom labels or captions.
5. Drawings should be labeled 'reduce to 70% of current size for publication'.

Currently, the following chemical drawing packages are acceptable: *ChemDraw* up to version 8.03, *Isis/Draw* up to version 2.5. *Macintosh: ChemDraw* up to version 8.03.

Color reproduction of *Figures* and/or formulae is possible. When any of the original graphics delivered with a manuscript are in color, it is assumed that the authors wish for them to be reproduced in color, unless otherwise specified in the cover letter. The authors must be prepared to bear the additional costs associated with color reproduction (the Editorial Office can provide an estimate of these charges upon request).

2.8. Chemical Equations and Physical or Mathematical Expressions. Chemical equations and physical or mathematical expressions should be numbered sequentially on the right-hand side with arabic numerals in parentheses. Physical quantities and variables that must be defined in the text should be written in *italics* (wavy line). The symbols proposed by IUPAC (cf. *Pure Appl. Chem.* **1979**, 51, 1) are recommended. Fractional expressions should be written with a slash, e.g., $h\nu/kT$.

3. Electronic Submission of Manuscripts

An electronic version of the manuscript should also be submitted. Submissions not in electronic form may face a delay in publication. *The following word-processing packages are currently accepted:* PC and compatibles: *MS Word* (up to version 2002), *WordPerfect* (up to version 2002). *Macintosh: MS Word* (up to version 2001). Publication of manuscripts prepared with these software packages may be facilitated, if the following guidelines are adhered to. Failure to adhere to these instructions may prevent all or part of the material supplied on disk from being used in production.

Hardcopy (in *triplicate*) of the manuscript is required for review. The disk should accompany the manuscript. The version on disk **must** exactly match the version of the hardcopy.

When preparing a manuscript, use the document mode or its equivalent in the word-processing program; *i.e.*, do not save files in 'Text Only' (ASCII) mode. If a non-Western version of the word-processing software was used to prepare the manuscript, save the file in Rich-Text Format (RTF). Do not include any page-layout instructions such as placement information for graphics in the file. The text should be left-justified, and automatic end-of-line hyphenation should be turned off. Use carriage returns only to end headings and paragraphs, not to break lines of text. Do not insert spaces before punctuation. References must conform to the format printed in the journal. Ensure that all characters are correctly represented throughout the manuscript: for example, 1 (one) and l (ell), 0 (zero) and O (Oh), X (ex) and \times (times sign). Check the final copy carefully for consistent notation and correct spelling. Check the disk with a virus-detection program. Disks containing viruses will not be processed. Label the disk with the manuscript name and the name of corresponding author. Additionally, platform, version of software used, and file names should be provided.

All text (including the title page, abstract, all sections of the manuscript, figure captions, scheme or chart titles and footnotes, and references) and tabular material should be in one file, with the complete text first, followed by the tabular material. It is best to use the fonts 'Times', 'Arial', and 'Symbol'. Some other fonts, particularly those that do not come bundled with the system software, may not translate properly. Ensure that all special characters (*e.g.*, Greek characters, math symbols, *etc.*) are present in the body of the text as characters and not as graphical representations. Tables created with a word processor's table format feature are preferred over those prepared in text mode. Ensure that each data entry is in its own table cell. If the text mode is used, separate columns with a single tab and use a line feed (return) at the end of each row.

Graphics, *e.g.*, figures, schemes, *etc.* should be provided on a separate diskette or CD. The file name for each image should be descriptive for the graphic. The preferred format is TIFF (Tagged Image File Format) at a resolution of at least 300 dpi. Since these files are rather large, they may also be compressed. Supported formats are: .zip, .hqx. HCA also accepts ZIP disks (100 MB) and CDs.

4. Nomenclature

All new compounds should be named in accordance with IUPAC rules (*cf. Appendix II*). As an additional guideline, the *Index Guide of Chemical Abstracts* should be consulted. Some special conventions peculiar to HCA are:

For common solvents, reagents, or other compounds, the molecular formulae or accepted abbreviations may be used: *e.g.*, CHCl_3 , NaCl, SOCl_2 , MeOH, DMF, DMSO, THF, Py. An *ad hoc* abbreviation may be used for a name or formula that occurs repeatedly. This has to be clearly defined, *e.g.*, THC = tetrahydrocannabinol.

Different alkyl or arylalkyl radicals should be designated with superscripted numbers: R^1 , R^2 , R^3 , *etc.* (Subscripts are used only to denote stoichiometry.) Aryl radicals should be designated by Ar^1 , Ar^2 , *etc.*, all others by X, Y, *etc.* (*e.g.*, X = O, Y = NH_2 , Z = Br).

Individual atoms should be referred to as C(2), N(5) (not C-2 and N-5), *etc.* For 'hydrogen atom attached to carbon atom 4', *etc.*, HCA prefers the notation H-C(4).

Some symbols and abbreviations are listed in *Appendix III*.

5. Units and Their Symbols

SI Units are to be used, especially in contributions dealing with physical chemistry. However, some non-SI units listed in *Appendix IV* are acceptable.

6. Special Instructions Concerning Contributions Containing X-Ray Crystal-Structure Results

All contributions which report the results of a crystal-structure determination, even in a minor way, must adhere to the following instructions.

It is the results of crystal-structure determinations which are of prime interest to readers of *HCA*. A detailed description of the experiment is not usually necessary, and only the pertinent crystallographic data need to be summarized in the experimental section. However, the full crystallographic data must be deposited in one of the crystallographic databases (see *d* below) **before** the manuscript is submitted. In addition, authors must validate their crystallographic data (see *c* below) and include the Validation Report with their manuscript. The manuscript will not be distributed to the referees until the database deposition numbers and Validation Reports for the reported crystal structures have been provided.

a) Information to be contained within the Discussion Section:

A labeled view of the molecule with **displacement ellipsoids, not arbitrary spheres**, will usually suffice, unless the authors specifically wish to discuss particular aspects of the structure or the experiment.

A brief description of the structure or any unusual features therein and a table of significant bond lengths, angles, or torsion angles may be given where appropriate to the discussion.

Full tables of refined atomic coordinates, bond lengths and angles, and related information will only be printed when *specifically* requested by the authors, and when the referees agree that the information is essential to the understanding of the discussion.

b) Information which must be contained within the Experimental Part:

A brief description of the procedures used for data collection, structure solution, and refinement. For routine analyses, this need not amount to more than a few sentences, but unusual parameters or procedures should be described. Crystallographic nomenclature and conventions should conform to the usage of *International Tables for Crystallography*. The following items should be given explicitly:

- Systematic name, *Chemical Abstracts* Reg. No., or other identifying name
- Source of material and solvent for crystallization
- Chemical formula
- Formula weight
- Crystal size
- Unit-cell dimensions and volume with standard uncertainties
- Crystal system and space group
- Number of molecules or formula units per unit cell
- Diffractometer used
- Radiation and wavelength
- Temperature and pressure of measurement (if different from 298 K and 1 atm)

- Calculated density D_x (and measured density, D_m , if applicable)
- Linear absorption coefficient
- Method of measuring intensities
- Max. value of $(\sin\theta)/\lambda$ or θ reached in intensity measurements
- Type of absorption correction applied (if applicable) and max. and min. values of correction
- Decay correction (if applicable) with maximum decay value
- Method used to solve and refine structure including treatment of H-atoms
- Use of F or F^2 magnitudes in least-squares refinement
- Number of measured, independent, and observed reflections
- Criterion for classifying reflections as observed [$I > n\sigma(I)$]
- Number of parameters refined
- Final values of $R(F)$ for the $I > n\sigma(I)$ reflections, wR (on F or F^2) for all reflections used in the refinement, and S (goodness-of-fit)
- Max. positive and max. negative electron density in final *Fourier* synthesis
- For polar structures, reason for choice of enantiomorph or method of testing absolute configuration
- All computer programs used

c) Validation of Crystallographic Data (to be done before submission of the manuscript)

In order to reduce the likelihood of incorrect or substandard crystal structures being reported, authors must test the validity of their crystal structure determinations prior to submission of their manuscript. The CIF ^{a)} for each structure in the paper can be uploaded to the IUCr's CHECKCIF facility at <http://journals.iucr.org/services/cif/checking/checkform.html> or validated locally with the program PLATON (downloadable from <http://www.cryst.chem.uu.nl/platon/> for details). Both these validation methods generate a Validation Report. Authors should examine the Validation Reports to ensure that no serious oversight has occurred with their crystal structure determinations (e.g. incorrect space group, seriously deficient data quality or structural model) and take appropriate corrective action if required. A copy of the final Validation Report for each structure in the paper must be submitted with the manuscript and any unresolved serious validation issues should be commented upon.

^{a)} Details concerning the Crystallographic Information File (CIF) format are available from *Acta Crystallogr., Sect A* **1991**, 47, 655 or the Web site <http://www.iucr.org/iucr-top/cif/index.html>

d) Deposition of Crystallographic Data (to be completed before submission of the manuscript)

Prior to submission of a manuscript, all crystallographic data must be deposited electronically in CIF format with the appropriate crystallographic database so that the referees can access the data.

The crystallographic data for **organic and organometallic** compounds should be deposited with the *Cambridge Crystallographic Data Centre (CCDC)* (see: <http://www.ccdc.cam.ac.uk>). Send your data in CIF format (excluding structure factors) by e-mail to deposit@ccdc.cam.ac.uk. The CCDC will provide the authors with one

deposition number for each structure by return e-mail. These deposition numbers should be included as a footnote in the manuscript by using the following standard text:

‘CCDC-..... contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via <http://www.ccdc.cam.ac.uk/conts/retrieving.html> (or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033; e-mail: deposit@ccdc.cam.ac.uk).’

The data for *inorganic* compounds should be deposited with the Fachinformationszentrum Karlsruhe (see: <http://www.fiz-informationsdienste.de/en/DB/icsd/depot.html>). Send your CIF by e-mail to crysdata@fiz-karlsruhe.de. A CSD number will be notified by return e-mail. The CSD number should be included as a footnote in the manuscript by using the following standard text:

‘Further details of the crystal structure investigation(s) may be obtained from the Fachinformationszentrum Karlsruhe, Informationsdienste, Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen, Germany, on quoting the depository number(s) CSD....’

7. Proofs and Corrections

Authors will be provided with two sets of proofs, one of which should be corrected and returned together with the edited manuscript to the editor within the indicated deadline. The author is solely responsible for checking the proofs.

Standard correction marks should be used. Corrections of errors other than those due to the printers or editors, or addition of new text, will be charged.

The author(s) should complete and return the keyword form provided with the proofs.

Keywords are entries in the annual subject index. Well-chosen keywords will help a reader to find articles of potential interest. Individual keywords should consist of not more than three words. Very general words or phrases (e.g., organic compounds, synthesis, instability, color, *etc.*) are clearly unsuitable as key words.