1. Instructions for Authors

Acta Chemica Iasi is published in two issues per year and is devoted to the publication of fundamental research papers in all fields of chemistry, material science, environmental (general) and education (general). Articles, Communications, Book Reviews, and Computer Software Reviews are published.

Manuscripts must be submitted by e-mail to: aci@chem.uaic.ro

Mailed hardcopy, fax submissions are not acceptable. Submission of a manuscript to *Acta Chemica Iasi* is contingent upon the agreement by all the authors that the reported work has not been previously published and that no part of this or any other closely related work is under consideration for publication elsewhere in any medium, including electronic journals, computer databases, and publicly accessible preprint Web sites.

Receipt of a manuscript for consideration will be acknowledged by the Editorial Office *via* e-mail. This acknowledgement will indicate the *manuscript reference number*, which must be quoted in all subsequent correspondence.

Authors are strongly encouraged to suggest the names and addresses of 3-5 suitable referees. Authors are requested not to suggest reviewers with whom they have a personal or professional relationship, especially if that relationship would prevent the reviewer from having an unbiased opinion of the work of the author. Recommendations of referees need not always be followed by the editors, who accept full responsibility for decisions regarding the manuscripts.

Book Reviews and **Computer Software Reviews** are prepared at the invitation of the Editor. Unsolicited reviews are not accepted.

Incomplete Manuscripts. Manuscripts that are incomplete at the time of submission must be revised to include the missing items or corrected files before peer review. The official date of receipt of the manuscript will be recorded as the date that the revised manuscript is received in the Editor's office in the complete and proper format.

Patent Activities and Intellectual Property Issues. Authors are responsible for ensuring that all patent activities and intellectual property issues are satisfactorily resolved.

Revised Manuscripts. When a revision is requested after peer review, the authors must return the revised manuscript promptly. One months after the request for revision of a Communication and two months after the request for revision of an Article, a revised manuscript will be handled as a new submission and will be given a new receipt date.

Proofs. The corresponding author of an accepted manuscript will receive e-mail notification and complete instructions when page proofs are available for review. The PDF proof made available for review is of publication quality so that authors may see a true representation of both the text and the graphics prior to Web and print publication. Page proofs should be checked carefully against the manuscript (in particular, all tables, figures, structures, captions, equations, and formulas, as well as clarity of the graphics), as this is not done by the Journal Publication until the author's changes have been made or the author's approval has been received. If a hardcopy of the page proof is returned, all corrections, revisions, and additions must be entered on the proof; if changes are returned via email, all corrections, revisions, and additions must be listed with their location clearly identified. Manuscripts for which page proofs are not returned in a timely manner will be withdrawn

from publication. Routine rephrasing of sentences or additions are not permitted at the page proof stage. Alterations should be restricted to serious changes in interpretation or corrections of data. Extensive or important changes on page proofs, including changes to the title or list of authors, are subject to Editorial review.

Manuscripts may be submitted in English and must be prepared with a word processor. Authors are requested to use the template document. Pages should be numbered consecutively beginning with the title page.

Manuscripts containing grammatical and/or stylistic deficiencies are handicapped during the review and editorial processes, leading to rejection or significantly longer publication times. Authors who are not fully fluent in English are strongly advised to gain assistance with manuscript preparation. 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", Dodd, J. S., Ed., 2nd edn., American Chemical Society: Washington, DC, 1997, or Strunk Jr., W. and White, E. B., "The Elements of Style", 4th edn., Prentice Hall: New York, 1999 (also found at http://www.bartleby.com/141/index.html).

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

2. General Considerations

2.1. Title Page

For the layout of the title page, a current issue of ACI should be consulted.

Attention is drawn to the following points:

a) The title of a manuscript, being of greatest importance for attracting readers' interest and for 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 with 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.

2.2. Abstract

An abstract in English should be provided. 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.

2.3. Keywords

For all types of manuscripts, 3 - 5 keywords, which best characterize the paper, should be given. For guidance, consult Chemical Abstracts General Subject Index.

2.4. Introduction

The introduction (no heading) should state briefly, with relevant references, the purpose of the investigation and its relation to other work in the appropriate field. All relevant citations should be included (see 2.8.).

2.5. Experimental

In the experimental section materials, methods and procedures should be described in this order, in sufficient detail to enable other chemists to repeat the experiments. The instruments used as well as measurement conditions and corresponding physical units should appear in a paragraph at the beginning of the Experimental section. Description of standard techniques applicable throughout the work should follow the paragraph on instrumentation. Novel experimental procedures should be described in detail, but procedures already published should merely be referred to by literature citation. General reaction conditions should be given only once. Both weight amounts and molar equivalents of all reactants and weight amounts and percentage yields of products should be included. Whenever possible, elemental analyses should be provided for new compounds. However, the molecular formula may be determined from physical data (e.g., high-resolution MS) if evidence of purity is presented.

2.6. Results and Discussion

Usually, the results are presented first, followed by a discussion of their significance. Only strictly relevant results should be given. The section may be further divided by subheadings. Equations, tables and figures should be used to shorten the text and make it readily understandable. Data should not be presented in duplicate.

2.7. Conclusion

The main conclusions of the study may be presented in a short Conclusions section, which may stand alone or form a subsection of a Discussion or Results and Discussion section.

2.8. References

References should be numbered sequentially in the order they are cited in the text. The numbers should be set superscript, usually after punctuation marks. Titles of journals must be abbreviated according to Chemical Abstracts (cf. Chemical Abstracts Service Source Index (CASSI) and Appendix II).

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) Surnames of authors should be followed by a comma and precede forename initials. Each initial is followed by a period and separated from the next by a space (unless hyphenated). A semicolon follows the set of initials.

Connectives should precede surnames, where appropriate; please distinguish whether or not they are capitalised (e.g. van or Van, el or El, d' or D'). Where a second part of a hyphenated forename (usually Japanese) has a lower-case style, only the first letter of the first part should be shown; e.g. Yamamoto, K., not Yamamoto, K.-i. Do not include jnr. or III etc. after authors' names.

Hyphenated forenames should show full punctuation (i.e. Dubois, J. E., not Dubois, J E.). Give proper contractions of Russian letters (Ya., Yu., etc.).

c) The name of the journal cited should be given in *Italics* and the journal volume numbers should be given in **Bold** (or the year, where there is no volume number). Note the required sequences: year, volume, pages for journals with a volume number; and year, pages for journals with no volume number.

d) 1. Composite references may be used, instead of a series of individual ones.

2. The use of the Latin terms ibid. and idem is not 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.

Examples of references to book chapters, books, patents, computer programs, and Ph. D. Theses, are also given.

References

1. Braverman, S.; Pechenick-Azizi, T.; Major, D. T.; Sprecher, M. Beta-halo-alpha, beta-unsaturated gamma-sultones. J. Org. Chem., 2007, 72, 6824-6831.

2. Krässig, H. A. In Cellulose Structure, Accessibility and Reactivity; Huglin, M. B., Ed.; Gordon and Breach Science Publishers, Yverdon, 1992; Vol. 11, pp. 6.

3. Dunitz, J. D. X-Ray Analysis and the Structure of Organic Molecules. Verlag Helvetica Chimica Acta: Basel, and VCH: Weinheim, 1995.

4. Kamata, T.; Wasada, N. Jap. Pat., 1990, 2-204469 pp. 381–384.

5. Sheldrick, G. M. SHELXL97, Program for the Refinement of Crystal Structures, University of Göttingen, Germany, 1997.

6. Peterson, B. R. Ph.D. Thesis, University of California, 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 Wasada15". If the reference carries the names of three or more authors it should be quoted as "Barbero et al.5", if Barbero is the first author, or as "Piscopo and co-workers1", if Piscopo is the senior author.

3. Preparation of the Manuscript - Detailed Information

3.1. Typesetting

Special types of print should be used as follows:

- **Boldface**: headings, designated numbers of chemical compounds.
- *Italics*: 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.
- SMALL CAPITAL: symbols of molar and normal concentrations (M and N), D and L, the names of the discoverer in the nomenclature of genera, species, or varieties.
- **Boldface italic**: the italicized terms and prefixes in headings.

An illustrative compilation of typesetting conventions is shown in Appendix I.

Use of hyphens

Hyphens should not be used for common two-word chemical composites, e.g. cation radical, radical anion, ion pair, hydroxy group, radical pair etc. However, composite adjectives should always be hyphenated, e.g. "the intimate ion-pair intermediate is one example of ion pairs that intervene"; "the transition state is as predicted by transition-state theory"; "the hydroxy group in this compound undergoes typical hydroxy-group reactions".

Series of words: if a series of words or compound names is given as a number of fore-terms and one stem-term, then the last complete word should be hyphenated accordingly, e.g. "methyl-, ethyl-, and nitro-benzene" (not nitrobenzene); "inter- and intra-molecular" (not intramolecular).

Spelling conventions

English (UK) should be used for word spelling.

3.2. 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 special character, such as *, +, \pm . Each footnote should be typed at the bottom of the page of the manuscript in which it is first mentioned. Footnotes must not be included with the references.

3.3. 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 and given suitable captions. 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.

3.4. Structural Formulae, Schemes, and Figures

Use Arabic <u>not</u> Roman numerals to denote structure numbers; these should be typed as bold face both in the structure blocks and in the text, and *should always be enclosed in parentheses*.

Since only a few characters can be conveniently set above "arrows" in reaction sequences, longer descriptions of reagents, etc., should be numbered (i), (ii), ... and collected together at the foot of the block with the identifying number set above the appropriate "arrow".

Pay particular attention to the conventions adopted in publications for the presentation of structures, i.e. (1) not (I) and (2) not (II) are appropriate, as described below.

Thus, partial bonds (electron delocalization) are shown by broken lines (). Stereochemistry of bonds is shown by dark wedges for "in front of page" and broken ones (narrowing with distance from the observer) for "behind page" bonds. Hydrogen bonds are shown dotted (....). For a benzene ring, a Kekulé structure should be used and not a hexagon containing a circle. Small alkyl substituents are denoted by Me, Et, etc. (not CH_3 , C_2H_5), Pr^i , Bu^t (with Roman superscripts italicised); *n*, *s*, *t* prefixes should be italicised (use of *tert* is discouraged).

Currently, the following chemical drawing packages are acceptable: ChemDraw up to version 11.0, or Isis/Draw up to version 2.5, ACD/ChemSketch up to version 11.0. For styles and drawing, follow this link: Chemicaldrawing

For authors using the *ChemDraw* program, the following preferences should be selected: bond spacing 15% of length, 8-pt *Helvetica* or *Arial* font for atom labels, 8-pt*Helvetica* or *Arial* font for captions, fixed length 14 pt (0.494 cm), bold width 2.0 pt (0.071 cm), line width 0.60 pt (0.021 cm), margin width 2.0 pt (0.071 cm), hash spacing 2.0 pt (0.071 cm). With appropriate margin settings, a maximum width of 12.5 cm should be created for structure blocks, schemes, and equations. Compound numbers should be in boldface type, but not atom labels or captions.

Figures that are subdivided into subfigures should have uniform designation with lower case letters, e. g. **1a** and **1b**.

Color reproduction of *Figures*, *Schemes* 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).

3.5. 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. The symbols proposed by *IUPAC - cf. Pure Appl. Chem.*, **51**, 1 (1979) - are recommended. Fractional expressions should be written with a slash, *e.g.*, *hv/kT*.

3.6. Nomenclature

All new compounds should be named in accordance with IUPAC rules (cf. Appendix III). As an additional guideline, the Index Guide of Chemical Abstracts should be consulted. The use of ACD/Name (version 11.0) or ACD/Name Chemist Version are recommended.

Some special conventions peculiar to Acta Chem. Iasi are:

For common solvents, reagents, or other compounds, the molecular formulae or accepted abbreviations may be used: *e.g.*, CHCl₃, NaCl, SOCl₂, 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.*, tetrahydrocannabinol (THC).

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 Ar¹, Ar², etc., all others by X, Y, etc. (e.g., X = O, Y = NH₂, 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., *ACI* prefers the notation H-C(4).

Some symbols and abbreviations are listed in Appendix IV.

3.7. 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 V are acceptable.

Appendices

- Appendix I
- Appendix II
- Appendix III
- Appendix IV
- Appendix V