

Pure and Applied Chemistry

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Introduction

Pure and Applied Chemistry is the official monthly Journal of IUPAC, with responsibility for publishing works arising from those international scientific events and projects that are sponsored and undertaken by the Union. The policy is to publish highly topical and credible works at the forefront of all aspects of pure and applied chemistry, and the attendant goal is to secure widespread acceptance of the Journal as an essential holding in academic and institutional libraries.

Pure Appl. Chem. publishes collections of papers based upon authoritative lectures presented at IUPAC sponsored events, most usually those of plenary or main lecturers. In exceptional circumstances, determined through prior negotiation, this may be extended to include selected contributions by a broader cross-section of participants. In addition, papers or collections of papers on topics of compelling scientific interest may be published by invitation or arrangement, as Special Topic features. Unsolicited manuscripts are not normally considered for publication.

Pure Appl. Chem. is also the designated medium for publication of recommendations, technical reports on standardization, recommended procedures, data compilations, and collaborative studies of IUPAC bodies.

Submission of Papers

Pure Appl. Chem. seeks to achieve representative, rapid and scientifically useful publication of Conference outputs. Accordingly, invited authors are urged to make every effort to participate and to submit manuscripts by the stated deadlines.

Manuscripts are to be submitted using the ManuscriptCentral online manuscript handling system. Authors will be given directions on how to access the system before the conference date (see below). A submission template and instructions are available on the Union's web site or can be obtained from the IUPAC Secretariat (E-mail: <edit.pac@iupac.org>). If you cannot use the submission template, follow the following instructions for setting up your file.

- Include all parts of the paper in a single file if possible.
- If illustrations are embedded in the document, also include them in separate files.
- Do not use the carriage return (enter) at the end of lines within a paragraph.
- Turn the hyphenation option off.
- Do not use the endnote feature for references.
- Do not number headings.
- Take care not to use l (ell) for 1 (one), O (capital o) for 0 (zero), or ß (German esszett) for β (beta).
- Use a tab, not spaces, to separate data points in tables.
- If you use a table editor function, ensure that each data point is contained within a unique cell; i.e., do not use carriage returns within cells.

Submission of a manuscript will be regarded as assurance that the same material is not being considered for publication by another journal.

Electronic file submission

Authors will receive an e-mail inviting them to submit a paper for consideration. If the 'accept' link is clicked, they will receive an e-mail providing them with a logon ID and temporary password to access ManuscriptCentral. They can then logon to their Author Center (<http://mc.manuscriptcentral.com/pac>) and continue the manuscript submission process. The link to an invited manuscript can be found under the list of "My Manuscripts" at the left side of the screen. Click on this link to complete the manuscript submission form. The information required includes keywords and the names of proposed reviewers. Complete address information for the principal Author and co-authors should be entered at this time. The online manuscript submission process can be interrupted at any point and resumed at a later time. After the manuscript has been submitted, its current status can be determined using ManuscriptCentral.

(Note: PDF files should only be submitted as an example of what the illustration or text looks like. Images in PDF files cannot be extracted for use in the print version.)

IUPAC Technical Reports and Recommendations

There are special requirements for deciding the category (Technical Report or Recommendations) to which a particular report belongs. Additional instructions can be found in the *IUPAC Handbook 2004-2005*:

- *Procedure for Publication of IUPAC Technical Reports and Recommendations*, or online as <www.iupac.org/reports/provisional/procedure.html>, and
- *Guidelines for Drafting IUPAC Technical Reports and Recommendations (2004)*, or online as <www.iupac.org/reports/provisional/guidelines.html>

These Guidelines contain more details than described in these general instructions, and authors are advised to consult these documents carefully before drafting an IUPAC report.

Preparation of Papers

A collection of papers based upon a Conference, Symposium or Workshop is expected to capture the scientific impact and topicality of the theme, and furnish readers with an indispensable archival resource. Conference papers are typically *short critical overviews of specialized topics*, and authors have considerable latitude in emphasizing review content or disclosing hitherto unpublished findings. *Pure Appl. Chem.* aspires to offer readers distinctive insights into new science that complement rather than compete or conflict with those published in the primary research literature.

A critical overview based upon a plenary presentation may occupy up to perhaps 12 Journal pages (at ~ 1000 words per page), whereas other forms of Conference presentation will usually be shorter (6 to 8 Journal pages), and may even incorporate a short experimental section to exemplify and underpin new findings. However guidelines on manuscript content and length are applied flexibly, and authors are welcome to explore the scope for departing from these guidelines, in consultation with the Scientific Editor.

Much emphasis is placed upon representative, rapid and scientifically useful publication of Conference outputs. Accordingly, invited authors are encouraged to make every effort to participate, and to adhere to the prescribed timetable for submission of manuscripts.

Abstract

Include a short abstract (not more than 200 words).

Illustrations

Illustrations will be reproduced in black and white only, unless the author pays for color

reproduction. If the figures are originally in color, be sure they can also be understood by the reader in black and white format (for example, do not refer to color elements in the caption).

Figures

Lettering, numbering, and symbols in the figures must be clear and suitable for reduction to single or double column width. Lettering and lines on graphs should also be strong enough to withstand reduction. Chemical schemes, etc., should be supplied as standard figures, and, in all cases, the figure must be accompanied by a title and/or legend that describes the illustration.

Figures should be numbered serially throughout the paper in arabic numerals and should be cited in the text at first occurrence. The word 'Figure' should be shortened to 'Fig.' at the beginning of figure captions and in the text, except where the word 'Figure' begins a sentence.

Structural formulas

Formulas should be prepared with particular care, preferably with a suitable computer program. They may be numbered with italic or underlined arabic numerals. Within reason, these numbers may be used in the text to avoid repetition of long chemical names. Structural formulas should be presented in groups where feasible to improve presentation and save space.

Tables

Tables should not be used more than is necessary and, in particular, they should not duplicate results that are presented in graphical form. Tables should be numbered serially throughout the paper in arabic numerals and should be cited in the text at first occurrence. Table headings should appear above the table with one line space between the heading and the table. The word 'Table' should be boldface, and the table heading should be typed with an initial capital for the first word and proper nouns only. If necessary, a font size smaller than 9 point may be used.

Mathematical expressions and chemical equations

Mathematical expressions and chemical equations should be indented on the left, with space above and below, and should be numbered in parentheses flush right.

$$k_p = A \exp(-E_A / RT) \quad (1)$$

Simple mathematical expressions should be left in the text, written in one line instead of in two-line form wherever possible to avoid awkward line spacing. Use additional half line spaces as needed to ensure that mathematical expressions in the text do not overlap preceding or succeeding lines.

For additional information on quantity calculus or quantity algebra and on percents and per mils, see IUPAC Interdivisional Committee on Terminology, Nomenclature and

Symbols, February 2002; available online at
<www.iupac.org/standing/ictns/quantity_and_percents.html>

Numbers

Numbers should be printed in roman (upright) fonts. Numerical values of physical quantities (and the symbols of units) should be printed in roman even in italic texts.

The decimal marker for IUPAC publications in English should be a point on the line. For many-digit numbers the digits should be grouped in threes around the decimal marker with a space* between the groups, but never leaving a single digit on its own.

Examples

Numbers in a running text: 3.1416 or 3.141 6

Numbers in a column:

1 000.234 5

21 110.216 48

500.123 3

Additional guidelines for the printing of numbers are detailed in the *Guidelines for Drafting IUPAC Technical Reports and Recommendations (2004)*, available in the *IUPAC Handbook 2004-2005* or online as
<www.iupac.org/reports/provisional/guidelines.html>

* *It is best to use a nonbreaking space of constant width (in MS Word under Windows, use ctrl-shift-space, or under Mac OS, use command-space), which also prevents the splitting of numbers on line breaks.*

References

All references should be mentioned in the text or captions. They should be typed in brackets, e.g., [41], in sequence. References appear at the end of the paper in numerical order. Inclusive page numbers are desirable.

Examples of formats are shown below. Abbreviations of journal titles should agree with usage by *Chemical Abstracts* (see *Chemical Abstracts Service Source Index, 1907-1994 Cumulative*, American Chemical Society, Columbus, Ohio, 1994).

Examples of Reference Formats:

1. J. P. Lee, G. C. Pimentel. *J. Chem. Phys.* **75**, 4241 (1981).
2. S. Stoeva, G. Grübler, H. Echner, W. Röspeck, W. Voelter. *Pure Appl. Chem.* **66**, 101-104 (1994). [Use names of all authors rather than *et al.*]
3. R. Stephenson. *Introduction to Nuclear Engineering*, p. 27. McGraw-Hill, New York (1964).
4. S. N. Loh, C.W. McNemar, J. L. Markley. In *Techniques in Protein Chemistry* (J. J. Villafranca, ed.), pp. 275-282. Academic Press, New York (1991).
5. F. Bloch. US Patent 2960 649, Filed 18 June 1954, Issued 15 Nov 1960.

Footnotes should be used sparingly and referred to in the text in parentheses as (Note a), etc. Only references to articles in journals, books, and issued patents will be permitted. Meeting abstracts and patent applications may not be quoted unless they are published in a form that is available for library reference.

Symbols and units

Symbols for scalar physical quantities (or variables) should be set in italic (sloping) type, and symbols for units, or labels, should be set in roman (upright) type. Quantity symbols may be qualified by subscripts or by further information in parentheses; subscripts should themselves be in italic type when they represent physical quantities, and otherwise in roman type. For other classes of quantities, (vectors, matrices, etc.) see additional information given below.

Quantity calculus should be used in presenting the values of physical quantities, and according to the following equation: (physical quantity) = (numerical value) x (unit). Each term in parentheses can be treated as an algebraic quantity. These two statements are necessary and sufficient to define quantity calculus. See the examples below and the IUPAC Green Book (ref. 1, list below) for further examples.

$$p = 0.123 \text{ mbar} = 12.3 \text{ Pa} = 12.3 \text{ N m}^{-2} \text{ or } p/\text{Pa} = 12.3$$
$$r = 2.13 \text{ \AA} = 0.213 \text{ nm} \text{ or } r/\text{nm} = 0.213$$
$$k = 10^{8.2} \text{ s}^{-1} \text{ or } \lg(k/\text{s}^{-1}) = 8.2$$

Note particularly the use of an italic font for quantity symbols such as p , r , and k , and the use of an upright font for unit symbols such as Pa, mbar, m, nm, and s. The format (quantity symbol)/(unit), as in $r/\text{nm} = 0.213$, is particularly convenient for heading the columns of tables and labeling the axes of graphs, so that the entries in the table columns or the labels on the tick marks of the graph may be pure numbers. The symbols lg and ln should be used for \log_{10} and \log_e , respectively. (For additional information, see *On the use of italic and roman fonts for symbols in scientific text*, I. M. Mills and W. V. Metanovski, IUPAC Interdivisional Committee on Nomenclature and Symbols, January 2000; available online at <www.iupac.org/standing/idcns/fonts_for_symbols.html>)

The following IUPAC references should be considered:

1. IUPAC Physical Chemistry Division, *Quantities, Units and Symbols in Physical Chemistry* (The IUPAC 'Green Book'); 2nd edition. Prepared for publication by I.M. Mills, T. Cvitaš, K.H. Homann, N. Kallay, and K. Kuchitsu. Blackwell Science, Oxford, UK (1993).
2. (a) IUPAC, *Compendium of Chemical Terminology: IUPAC Recommendations* (The IUPAC 'Gold Book'); 2nd edition. Compiled by A.D. McNaught and A. Wilkinson, Blackwell Science, Oxford, UK (1997); (b) Gold Book online edition: www.iupac.org/publications/compendium/index.html

3. (a) IUPAC Commission on the Nomenclature of Inorganic Chemistry, *Nomenclature of Inorganic Chemistry. Recommendations 1990* (The IUPAC 'Red Book'). G. J. Leigh (Ed.). Blackwell Scientific Publications, Ltd., Oxford, UK (1990). (b) IUPAC Commission on the Nomenclature of Inorganic Chemistry, *Nomenclature of Inorganic Chemistry I, Recommendations 2000* (The IUPAC 'Red Book II'). J. A. McCleverty and N. G. Connelly (Eds.). Royal Society of Chemistry, Cambridge, UK (2000).
4. IUPAC Commission on the Nomenclature of Organic Chemistry, *Nomenclature of Organic Chemistry* (The IUPAC 'Blue Book'); Sections A, B, C, D, E, F, and H. Prepared for publication by J. Rigaudy and S. P. Klesney, Pergamon Press, Oxford, UK (1979).
5. IUPAC Commission on the Nomenclature of Organic Chemistry, *A Guide to IUPAC Nomenclature of Organic Compounds*. R. Panico, W. H. Powell, J.-C. Richer (Eds.). Blackwell Scientific Publications, Ltd., Oxford, UK (1993).
6. IUPAC Commission on Macromolecular Nomenclature, *Compendium of Macromolecular Nomenclature* (The IUPAC 'Purple Book'). Prepared for publication by W. V. Metanomski. Blackwell Scientific Publications, Ltd., Oxford, UK (1991).
7. IUPAC Analytical Chemistry Division, *Compendium of Analytical Nomenclature* (The IUPAC 'Orange Book'); 3rd edition. Prepared for publication by J. Inczédy, T. Lengyel, A. M. Ure. Blackwell Science, Ltd., Oxford, UK (1998).
8. D.R. Lide, Jr. Use of abbreviations in the chemical literature, *Pure Appl. Chem.* **52**, 2229-2232 (1980).

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