

J. Synchrotron Rad. (2000). **7**, 47–51

Notes for Authors

1. Scientific scope

The *Journal of Synchrotron Radiation* seeks to cover all aspects of synchrotron radiation thus bringing together the full range of interests and skills of the synchrotron radiation community. Contributions are invited within the general areas of instrumentation, methods and applications. Instrumentation papers covering synchrotron radiation sources and beamlines, optics, detectors, electronics and data acquisition, and sample chambers and environment are welcomed. Methods and applications papers are invited within the categories of diffraction, spectroscopy and imaging.

2. Categories of contributions

Contributions should conform to the general editorial style of the journal.

2.1. Research Papers

Full-length *Research papers* should not normally exceed the equivalent of about 10000 words.

2.2. Short Communications

Short Communications are intended for the presentation of topics of limited scope or for preliminary announcements of novel research findings. They are not intended for interim reports of work in progress, and must report results that are of scientific value in their own right.

Short Communications should not exceed two journal pages (about 1500 words). A maximum of two figures and two tables of appropriate size are permitted. They are sent to referees in the normal way.

2.3. Fast Communications

Fast Communications should not normally exceed the equivalent of about 2000 words. In the letter accompanying the submission, authors should state why rapid publication is essential. Papers submitted for the *Fast Communications* section but judged by the editor not to merit rapid publication will be considered for inclusion with regular papers.

2.4. Reviews

The Main Editors occasionally invite leaders in selected areas to write *Lead Articles*, which are forward-looking reviews of specific topics. In addition, unsolicited review articles may be submitted. A brief outline of the proposed article should first be sent to one of the Main Editors. All selected *Lead Articles* and review articles will be refereed in the usual manner. These articles should not normally exceed 15000 words.

2.5. Computer Programs

A brief description of the purpose, strategy, computer language, machine requirements, input requirements and the type of results obtained should be included. It is also ordinarily required that the adequacy of the documentation shall have been proven by the

successful use of the program by someone outside the author's institution. *Computer Programs* should not normally exceed 5000 words. They are sent to referees in the normal way.

2.6. Laboratory Notes

These are very brief descriptions of special devices, equipment modifications, techniques for accomplishing certain tasks *etc.* A simple schematic drawing may often be preferable to an actual photograph of the apparatus. These articles should not normally exceed 500 words and will not be refereed.

2.7. Computer Program Abstracts

This section provides a rapid means of communicating up-to-date information concerning both new programs or systems and significant updates to existing ones. Either the names and addresses of those people outside the author's laboratory who have used and tested the program(s) or a source-code listing and test execution should be provided. These will be sent to the referees as supporting material but will not be published or deposited in any form. A *Computer Program Abstract* should not exceed 500 words in length and should use the standard format given in *J. Appl. Cryst.* (1985), **18**, 189–190.

2.8. Letters to the Editor

These may deal with non-technical aspects of synchrotron radiation, its role, its propagation, the proper functions of its Societies *etc.* or may make a technical observation that would usefully be brought to wider attention.

2.9. New Commercial Products

Announcements of new commercial products are published free of charge. The descriptions, up to 300 words or the equivalent if a figure is included, should give the manufacturer's full address.

2.10. Synchrotron Radiation Meetings and Short Courses

This section contains details of meetings of scientific societies, congresses, summer schools *etc.* that are of interest. Contributions should be sent to the Editorial Office in Chester.

3. Submission and handling of manuscripts

3.1. Address for submissions

All papers should be sent to:

The Managing Editor
International Union of Crystallography
5 Abbey Square
Chester CH1 2HU
England

Telephone: 44 1244 342878

Fax: 44 1244 314888

E-mail: med@iucr.org

Ftp: [ftp.iucr.org](ftp:iucr.org) (192.70.242.1)

3.2. Submission

Manuscripts and figures should be prepared using the file formats listed in §3.9. Three paper copies and the electronic file(s) should be submitted; authors are reminded to keep an exact copy of the submission for later editorial adjustments and for checking proofs.

On acceptance, an electronic version of the final manuscript will be required by the Editorial Office.

Contact details for the editors are available at <http://journals.iucr.org/s/services/editors.html>. Editors are assigned to a paper according to their current workload and expertise. However, authors should indicate, in their covering letter, the name of their preferred editor.

3.3. Languages of publication

The languages of publication are English, French, German and Russian.

3.4. Handling of manuscripts

The Co-editor to whom the manuscript is assigned is responsible for choosing referees and for accepting or rejecting the paper. This responsibility includes decisions on the final form of the paper and interpretation of these Notes when necessary.

If changes to a manuscript requested by the editorial staff or the Co-editor are not received within **two months** of transmittal to the author, the submission will automatically be withdrawn. Any subsequent communication of the material will be treated as a new submission in the editorial process.

For accepted papers, it is the responsibility of the Managing Editor to prepare the paper for printing. This may involve correspondence with the authors and/or the responsible editor in order to resolve ambiguities or to obtain satisfactory figures or tables. The date of acceptance that will appear on the published paper is the date on which the Managing Editor receives the last item required. Correspondence will be sent to the author who signed the letter of submission unless the Managing Editor is informed of some other suitable arrangement.

On rare occasions, an editor may consider that a paper is better suited to another IUCr journal. Alterations to the journal of publication will only be made after full discussion with the communicating author.

3.5. Author's warranty

The submission of a paper is taken as an implicit guarantee that the work is original, that it is the author(s) own work, that all authors concur with and are aware of the submission, that all workers involved in the study are listed as authors or given proper credit in the acknowledgments, that the manuscript has not already been published (in any language or medium), and that it is not being considered and will not be offered elsewhere while under consideration for an IUCr journal.

3.6. Copyright

Except as required otherwise by national laws, an author must sign and submit a copy of the Transfer of Copyright Agreement form for each manuscript before it can be accepted.

3.7. Author grievance procedure

An author who believes his paper has been unjustifiably treated by the Co-editor may appeal to one of the Main Editors for a new review.

3.8. Contact e-mail address

The contact author must provide an e-mail address for editorial communications and despatch of electronic proofs.

3.9. File format, naming and transfer

The manuscript should be prepared using T_EX, L^AT_EX or Word. Authors are encouraged to use the templates available from the Editorial Office by e-mail (med@iucr.org) or by ftp (from the 'templates' directory). All Word submissions should be accompanied by an RTF (rich text format) file.

Figures may be sent in PostScript, encapsulated PostScript or TIFF formats. The resolution of bitmap graphics should be a minimum of 1200 d.p.i.

All files need to be given a filename constructed from the *reference number* supplied by the Co-editor. Files containing text in T_EX or L^AT_EX should be given the extension `.tex`, Word files should be given the extension `.doc` and RTF files `.rtf`. Illustrations in PostScript, encapsulated PostScript or TIFF format should be given the extensions `.ps`, `.eps` or `.tif`, respectively. Multiple files for the same submission should be identified by filenames constructed as `ref.id.ext` where *id* indicates the contents, e.g. `xz1087.fig1.ps` and `xz1087.fig2.ps`.

After acceptance, the final version of the paper should be sent to the Editorial Office by e-mail (med@iucr.org), on diskette or (for files larger than 70K bytes) by ftp as described below.

(i) On your workstation enter:	<code>ftp ftp.iucr.org</code>
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(v) Transfer a file from your account (e.g. <code>j29.ps</code>) as an identifiable name (e.g. <code>ja0325.ps</code>):	<code>put j29.ps ja0325.ps</code>
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(vii) Finish off the ftp session by entering:	<code>bye</code>
(viii) Send an e-mail to Chester (med@iucr.org) with a list of the files transferred by ftp.	

4. Abstract, synopsis and keywords

All scientific contributions must be preceded by an English language *Abstract* and a one or two sentence *Synopsis* of the main findings of the paper for inclusion in the Table of Contents. The *Abstract* should state concisely the principal results obtained.

The *Abstract* should be suitable for reproduction by abstracting services without change in wording. It should not repeat information given in the title. Ordinarily 200 words suffice for *Abstracts* of a full-length article and 100 words for shorter contributions. It should make no reference to tables, diagrams or formulae contained in the paper. It should not contain footnotes. Numerical information given in the *Abstract* should not be repeated in the text. It should not include the use of 'we' or 'I'.

Literature references in an *Abstract* are discouraged. If a reference is unavoidable, it should be sufficiently full within the *Abstract* for unambiguous identification, e.g. [Smith (1998). *J. Synchrotron Rad.* **5**, 21–31].

Authors should ideally supply at least five keywords.

5. Diagrams and photographs ('figures')

Figures should be prepared using one of the file formats listed in §3.9. Hard-copy figures must be provided in all cases.

The choice of tables and figures should be optimized to produce the shortest printed paper consistent with clarity. Duplicate presentation of the same information in both tables and figures is to be avoided, as is redundancy with the text. In a paper only those

figures which are strictly necessary to illustrate the techniques or results described will be published: any others will be deposited. The text should be adequate to give the remaining information.

In papers which use powder profile fitting or refinement (Rietveld) methods, figures which present the experimental and calculated diffraction profiles of the material studied should also contain the difference profile. As primary diffraction data cannot be satisfactorily extracted from such figures, the basic digital diffraction data should be deposited (see §11.3)

5.1. Quality

Hard-copy greyscale or colour images should be provided as glossy prints; laser printer or photocopier output will generally be unsatisfactory for reproduction of such diagrams. High-resolution laser printer output is satisfactory for line drawings.

5.2. Size

Diagrams should be as small as possible consistent with legibility. They will normally be sized so that the greatest width including lettering is less than the width of a column in the journal.

5.3. Lettering and symbols

Fine-scale details and lettering must be large enough to be clearly legible (ideally 1.5–3 mm in height) after the whole diagram has been reduced to one column width.

Lettering should be kept to a minimum; descriptive matter should be placed in the legend.

5.4. Numbering and legends

Diagrams should be numbered in a single series in the order in which they are referred to in the text. A list of the legends ('figure captions') should be included in the manuscript.

5.5. Colour figures

Figures in colour are accepted at **no cost to the author** provided that the editor agrees that they improve the understanding of the paper.

6. Tables

Tables produced in Word should be prepared using the Word table editor.

6.1. Economy in use of tables

Numerical information is generally most economically presented in tables. Text and diagrams should not be redundant with the tables.

6.2. Design, numbering and size

Tables should be numbered in a single series of arabic numerals in the order in which they are referred to in the text. They should be provided with a caption.

Tables should be carefully designed to occupy a minimum of space consistent with clarity.

7. Mathematics and letter symbols

Authors submitting in Word should use the Word equation editor to prepare displayed mathematical equations.

The use of the stop (period) to denote multiplication should be avoided except in scalar products. Generally no sign is required but, when one is, a multiplication sign (\times) should be used.

Vectors should be in bold type and tensors should be in bold-italic type.

Greek letters should not be spelled out.

Care should be taken not to cause confusion by using the same letter symbol in two different meanings.

Gothic, script or other unusual lettering should be avoided. Another typeface may be substituted if that used by the author is not readily available.

Equations, including those in published Appendices, should be numbered in a single series.

8. Multimedia

Multimedia additions to a paper (*e.g.* time-lapse sequences, three-dimensional structures) are welcomed; they will be made available via *Crystallography Journals Online*.

9. Nomenclature

9.1. Crystallographic nomenclature

Authors should follow the general recommendations produced by the IUCr Commission on Crystallographic Nomenclature (see reports at <http://www.iucr.org/iucr-top/comm/cnom/>).

Atoms of the same chemical species within an asymmetric unit should be distinguished by an appended arabic numeral. **Chemical and crystallographic numbering should be in agreement wherever possible.** When it is necessary to distinguish crystallographically equivalent atoms in different asymmetric units the distinction should be made by lower-case roman numeral superscripts (*i.e.* i, ii, iii *etc.*) to the original atom labels. Other details should conform with *Acta Crystallographica* [*Acta Cryst.* (1998), **A54**, 1–6].

9.2. Nomenclature of chemical compounds *etc.*

Names of chemical compounds and minerals are not always unambiguous. Authors should therefore quote the chemical formulae of the substances dealt with in their papers.

Chemical formulae and nomenclature should conform to the rules of nomenclature established by the International Union of Pure and Applied Chemistry (IUPAC), the International Union of Biochemistry and Molecular Biology (IUBMB), the International Mineralogical Association and other appropriate bodies. As far as possible the crystallographic nomenclature should correspond to the systematic name.

Any accepted trivial or nonsystematic name may be retained, but the corresponding systematic (IUPAC) name should also be given.

9.3. Units

The International System of Units (SI) is used except that the ångström (symbol Å, defined as 10^{-10} m) is generally preferred to the nanometre (nm) or picometre (pm) as the appropriate unit of length. Recommended prefixes of decimal multiples should be used rather than ' $\times 10^n$ '.

10. References

References to published work must be indicated by giving the authors' names followed immediately by the year of publication,

e.g. Neder & Schulz (1998) or (Neder & Schulz, 1998). Where there are three or more authors the reference in the text should be indicated in the form Smith *et al.* (1998) or (Smith *et al.*, 1998) *etc.* (all authors should be included in the full list).

At the end of the paper a list giving full details of all references should be appended separately. In the reference list, entries for journals [abbreviated in the style of *Chemical Abstracts* (the abbreviations *Acta Cryst.*, *J. Appl. Cryst.* and *J. Synchrotron Rad.* are exceptions)], books, multi-author books, computer programs, personal communications and undated documents should be arranged alphabetically and conform with the style shown below.

Sample reference list

- Andrews, M., Wright, H. & Clarke, S. A. (1998). In preparation.
 Bürgi, H.-B. (1989). *Acta Cryst.* **B45**, 383–390.
 Ferguson, G., Schwan, A. L., Kalin, M. L. & Snelgrove, J. L. (1997). *Acta Cryst.* **C53**, IUC9700009.
 Hervieu, M. & Raveau, B. (1983a). *Chem. Scr.* **22**, 117–122.
 Hervieu, M. & Raveau, B. (1983b). *Chem. Scr.* **22**, 123–128.
 International Union of Crystallography (1998). (*IUCr Journal of Synchrotron Radiation*, <http://www.iucr.org/jsr>).
 Jones, P. T. (1987). Personal communication.
 McCrone, W. C. (1965). *Physics and Chemistry of the Organic Solid State*, Vol. 2, edited by D. Fox, M. M. Labes & A. Weissberger, pp. 725–767. New York: Interscience.
 Perkins, P. (undated). PhD thesis, University of London, England.
 Sheldrick, G. M. (1976). *SHELX76. Program for Crystal Structure Determination*. University of Cambridge, England.
 Smith, J. V. (1988). *Chem. Rev.* **88**, 149–182.
 Smith, J. V. & Bennett, J. M. (1981). *Am. Mineral.* **66**, 777–788.
 Vogel, A. (1978). *Textbook of Practical Organic Chemistry*, 4th ed. London: Longman.

Note that **inclusive** page numbers must be given.

11. Supplementary publication procedure (deposition)

11.1. Purpose and scope

Parts of some papers are of interest to only a small number of readers, and the cost of printing these parts is not warranted. Arrangements have therefore been made for such material to be deposited with the IUCr electronic archive, with the Protein Data Bank, the Nucleic Acid Database and the ICDD as appropriate.

11.2. IUCr electronic archive

All material for deposition in the IUCr electronic archive should be supplied electronically.

Non-structural information, which may include:

- details of the experimental procedure;
- details of the stages of structure refinement;
- details of mathematical derivations given only in outline in the main text and in mathematical Appendices;
- lengthy discussion of points that are not of general interest or that do not lead to definite conclusions but that do have significant value;

additional diagrams,

should be supplied in one of the formats given in §3.9.

Structural information (for small-molecule structures) should be supplied in CIF format; structure factors should be supplied as .fcf files.

11.3. Powder diffraction data

For papers that present the results of powder diffraction profile fitting or refinement (Rietveld) methods, the primary diffraction data, *i.e.* the numerical intensity of each measured point on the profile as a function of scattering angle, will be deposited.

11.4. Macromolecular structures

Authors should follow the deposition recommendations of the IUCr Commission on Biological Macromolecules. For all structural studies of macromolecules, coordinates and structure factors must be deposited with the Protein Data Bank or the Nucleic Acid Database if a total molecular structure has been reported. Authors must supply the Protein Data Bank/Nucleic Acid Database reference codes before the paper can be published.

11.5. XAFS data

For papers that present XAFS data of an unknown system, the deposition of primary $\chi(K)$ data will be encouraged.

11.6. Other spectroscopic, diffraction and imaging data

Deposition of primary data is generally encouraged. Please enquire prior to submission as regards preferred format.

12. Crystallography Journals Online

Full details of author services can be found at <http://journals.iucr.org/s/services/authorservices.html>.

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Authors may obtain information about the current status of their papers at <http://journals.iucr.org/services/status.html>.

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