

Notes for Authors – Journal of Synchrotron Radiation

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

2.1. Full Articles

Full Articles should not normally exceed the equivalent of about 10 000 words (1000 words are equivalent to about four pages of double-spaced manuscript). All papers are sent to referees (ordinarily two) before they are accepted for publication.

2.2. Short Communications

These 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 differ from ordinary articles not only in being shorter (they should not normally exceed 1000 words), but also in being printed in smaller type. They are sent to referees in the normal way.

2.3. 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 15 000 words.

2.4. 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.

2.5. 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.

2.6. 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. Reprints of this paper may be obtained from the Managing Editor.

2.7. 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.

2.8. 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.

The International Union of Crystallography can assume no responsibility for the accuracy of the claims made.

2.9. 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 should be prepared on one side of the paper in **double-spaced** format. All contributions should be submitted in **triplicate** and authors are reminded to keep an exact copy of the original and revised manuscript for later editorial adjustments and for checking proofs. A machine-readable version of the final accepted manuscript will be requested by the Editorial Office, provided it can be prepared using one of the four word-processing formats listed in §3.5. This request is designed to reduce publication times.

Every issue of the journal contains the names and addresses of the Main Editors and the Co-editors. This information is also

available at <http://www.iucr.org/jsr.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 or Russian. All contributions must be accompanied by an English language *Abstract*.

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 three 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. Proofs 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. File formats

A machine-readable version of the paper should be prepared in \TeX , \LaTeX , WordPerfect 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). It would be appreciated if all Word submissions were accompanied by an RTF (rich text format) file. After acceptance of the paper for publication, authors should send the version of the paper accepted by the Co-editor to the Editorial Office by e-mail or ftp (see §11), or on diskette.

3.6. 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 acknowledgements, 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. For these reasons, the submission must be made over the signature of at least one author.

3.7. Copyright

Except as required otherwise by national laws, an author must sign and submit a copy of the Transfer of Copyright Agreement form (given in at the end of these Notes) for each manuscript before it can be accepted.

3.8. 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.

3.9. Contact e-mail address

The contact author should, where possible, provide an e-mail address. This will be used for editorial communications and will normally appear in the published paper.

4. Layout and typography

Contributions should be prepared on one side of the paper in **double-spaced** format with wide margins, and should conform to the general editorial style of IUCr journals.

4.1. Type style

The editorial staff in Chester will indicate to the printer the style of type to be used. However, it is helpful if authors indicate vectors and tensors by a wavy underline.

4.2. Mathematics and letter symbols

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.

Greek letters should not be spelled out except in marginal notes of clarification.

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 identified in marginal notes. The printer may be instructed by the Managing Editor to use another type face if that indicated by the author is not readily available.

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

5. Abstract, synopsis and keywords

All scientific contributions must be accompanied 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 for the relevant issue. 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 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.

6. Diagrams and photographs ('figures')

6.1. Design

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.

Supplementary diagrams may be deposited (see §10.1).

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 §10.3).

6.2. Quality

Diagrams must be provided in 'hard-copy' form, that is, as careful drawings in black ink or as high-quality photographic copies (glazed prints, not mounted). An individual hard-copy diagram must be provided for each figure.

6.3. 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. They should be provided as glossy prints or slides; laser printer or photocopier output will generally be unsatisfactory for colour reproduction. Slides should be accompanied by a photocopy showing the required figure layout.

6.4. Size

Diagrams should be as small as possible consistent with legibility. If possible, each diagram should be provided on a separate sheet of about A4 International Paper Size (210 × 297 mm). They will normally be further reduced by the printer, generally so that the greatest width including lettering is less than the width of a column of the journal (approximately 85 mm). Figures at greater than column width are allowed at editorial discretion.

6.5. Lettering and symbols

Fine-scale details and lettering must be large enough to be clearly legible (not less than 1.2 mm in height) after the whole diagram has been reduced to one column (85 mm) width.

Lettering should be kept to a minimum; quantitative data should be given as tables and descriptive matter should be placed in the legend.

6.6. Numbering and legends

Diagrams and photographs must be numbered as figures in a single series, normally in the order in which they are referred to in the text. A list of the legends ('figure captions') is to be attached to the manuscript.

6.7. Electronic submission of figures

After acceptance of the paper for publication, authors may send figures direct to the Editorial Office by e-mail or ftp (see §11).

Figures may be sent in HPGL, PostScript, encapsulated PostScript or TIFF formats. The resolution of bitmap graphics should be 1200 d.p.i. Hard-copy figures must be provided in all cases.

7. Tables

7.1. Economy in use of tables

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

Small tables will normally be set in type while large tables may be photographically reproduced or deposited.

7.2. Design, numbering and size

Tables must be numbered in a single series of arabic numerals, normally in the order in which they are referred to in the text. They should be provided with a caption either at the top or, if the table is to be photographed, on a separate sheet.

Tables should be carefully designed to occupy a minimum of space consistent with clarity. Tables to be photographed should be prepared in single spacing, without excessive space between columns.

8. Nomenclature

8.1. Crystallographic nomenclature

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].

Authors are encouraged to follow the recommendation of the International Organization for Standardization (ISO) and use the term standard uncertainty, abbreviated s.u., in place of the traditional term estimated standard deviation [see Schwarzenbach *et al.* (1995), *Acta Cryst.* **A51**, 565–569]. The standard uncertainty should be expressed as a number in parentheses following the numerical result and should be on the scale of the least significant digits of the result.

Anisotropic displacement parameters should be reported as *U* values with the indices *ij* given as superscripts [see Trueblood *et al.* (1996), *Acta Cryst.* **A52**, 770–781].

8.2. 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.

If help on assigning systematic names is sought from advisory sources, authors are requested to indicate the source consulted.

8.3. 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 ' $\times 10^n$ '.

9. 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*), 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/jrsr.html>.
 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.

When more than ten references are taken from a data base (usually for a structural paper), a condensed reference notation of the Coden type should be used.

10. Supplementary publication procedure (deposition)

10.1. 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, the Brookhaven Protein Data Bank and the ICDD as appropriate.

Authors are encouraged to submit material for deposit in electronic format. The information to be deposited is **at the discretion of the Co-editor** and may include:

- Details of the experimental procedure.
- Details of the stages of structure refinement.
- Primary data for techniques such as XAFS.
- 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.

All material to be deposited should be clearly so marked; it will be subject to the usual refereeing procedure.

10.2. Preparation of material for deposit

Hard-copy material for deposit should:

- be of a quality such that photocopies of it are completely legible;
- have dimensions for text and tables not exceeding A4 International Paper Size (210 × 297 mm) (larger dimensions may be acceptable in exceptional circumstances);
- not be photographically reduced so that character heights are less than 1.2 mm;
- contain the title page of the paper to which it relates (including the *Abstract*);
- have pages clearly numbered to ensure the correct sequence;
- be sent **in triplicate** with the paper when it is submitted.

After acceptance of the paper for publication, material for deposition may be sent direct to the Editorial Office by e-mail or ftp (see §11).

10.3. 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.

Co-editors will send X-ray powder diffraction data (reported either in the paper or in the deposited material) to the International Centre for Diffraction Data (ICDD), 12 Campus Boulevard, Newtown Square, PA 19073-3273, USA. These data will then be checked and assigned an ICDD reference number which will, where possible, be published in the paper.

10.4. Macromolecular structures

Data deposited should correspond to the level of detail described in the structural paper. For all structural studies of macromolecules, coordinates and structure factors must be deposited with the Protein Data Bank at Brookhaven National Laboratory if a total molecular structure has been reported. Authors should supply the Protein Data Bank reference codes for inclusion in the published paper.

An author may request that the structure factors be given a privileged status for a period of no longer than four years and for atomic coordinates no longer than one year from the date of publication. Earlier release would require the specific consent of the author.

10.5. XAFS data

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

10.6. Other spectroscopic, diffraction and imaging data

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

11. File transfer

After acceptance of the paper for publication, authors with computer access to the Internet may use anonymous file transfer protocol (ftp) to transfer large electronic files to the Editorial Office in Chester. Files larger than 70K bytes should be transferred in this way, smaller files can be sent by e-mail to **med@iucr.org**.

The procedure for transferring files by ftp is described below. Files need to be deposited in a directory called 'incoming/s' with a filename constructed from the *reference number* assigned to the

File transfer procedure

- (i) On your workstation enter: `ftp ftp.iucr.org`
- (ii) Wait for **Name ...:** prompt and enter: `anonymous`
- (iii) Wait for **Password:** prompt and enter: `your e-mail address`
- (iv) Wait for `ftp>` prompt and enter: `cd incoming/s`
- (v) Transfer a file from your account (e.g. `j29.ps`) as an identifiable name (e.g. `ja0325.ps`): `put j29.ps ja0325.ps`
- (vi) Wait for `ftp>` prompt before sending another file
- (vii) Finish off the ftp session by entering: `bye`
- (viii) Send an e-mail to Chester (`med@iucr.org`) with a list of the files transferred by ftp

paper. Files containing text in $\text{T}_{\text{E}}\text{X}$ or $\text{L}_{\text{A}}\text{T}_{\text{E}}\text{X}$ should be given the extension `.tex`, WordPerfect or Word files should be given the extensions `.wp` or `.doc`, respectively, and RTF files `.rtf`. Files containing diagrams in HPGL, PostScript, encapsulated PostScript or TIFF format should be given the extensions `.hpg`, `.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`.

The procedure for transferring files is summarized in the box opposite.

12. Electronic status information

Authors may obtain information about the current status of their papers *via* the world-wide web at the address <http://www.iucr.org/docs/status.html/> (authors will need to provide the Co-editor reference number of their paper and the last name of one of the authors) or by e-mail by sending an e-mail message to `status@iucr.org` with the Co-editor reference number and the name of one of the authors as the subject line (e.g. `JA0325 Smith`). The body of the message should be empty. A status report will be returned by e-mail.

13. Reprints

Twenty-five reprints of each published article will be provided to a nominated author free of charge.

International Union of Crystallography – Transfer of Copyright Agreement

Title of Article *(Please type or use capital letters)*

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Authors *(Please type or use capital letters)*

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- (1) All proprietary rights other than copyright, such as patent rights.
- (2) The right to use all or part of this article in future works prepared by or on the behalf of the author.
- (3) In the case of 'work for hire', the right of the employer to incorporate all or part of this article in future works.
- (4) The royalty-free right of the employer to make copies of this article, without further permission, for his or her own use but not for resale. Any identification or notice appearing on the pages to be reproduced must not be deleted.

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Signature

Name and position, if not author

Name and position, if not author

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Date

Date

This Transfer of Copyright Agreement must be signed by at least one of the authors (who agrees to inform the others, if any) or, in the case of a 'work made for hire', by the employer.

By signing this form you certify that your contribution is your original work, has not been published before (in any language or medium) and is not being considered for publication elsewhere; that you have obtained permission for and acknowledged the source of any excerpts from other copyright works; and that to the best of your knowledge your paper contains no statements which are libellous, unlawful or in any way actionable.

The signed statement must be received before the article can be accepted for publication. Requests for further information should be sent to the Executive Secretary of the Union.

* In this case please give further details overleaf.

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M. E. Ref.	Co-editor Ref.	Issue	Journal
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