Journal of
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Notes for authors 2005

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 refereed 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 15000 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. Authors would usually be expected to be those who developed the program. *Computer Programs* should not normally exceed 5000 words. They are refereed 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. Authors would usually be expected to be those who developed the program. 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.

2.7. Teaching and Education

Papers in this category cover all aspects of an educational nature related to the general field of synchrotron radiation. All contributions should be submitted to one of the Main Editors.

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 or scientific comment 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. Meeting Reports

These are normally invited. Prospective authors interested in writing such items should first contact one of the Main Editors.

2.11. 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.

2.12. Obituaries

These will be commissioned by the Main Editors.

3. Submission and handling of manuscripts

3.1. Submission

Full details of the submission procedure can be found at **http://journals.iucr.org/s/services/submitbdy.html**. On initial submission, the article should be prepared as a single file (PDF, Word or RTF, PostScript, or encapsulated PostScript). Authors are encouraged to use the templates available from **http://journals.iucr.org/s/services/helpsubmit.html** or from the Editorial Office by e-mail (**med@iucr.**

org) or by ftp (from the 'templates' directory). Full instructions for submitting a paper are given at **http://journals.iucr.org/s/services/submitinstructions.html**. After acceptance, source files of the article (see §3.8) should be uploaded.

In the case of Addenda or Errata to published papers, the article should be submitted to the Co-editor of the original paper.

3.2. Languages of publication

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

3.3. 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 a Main Editor, Co-editor or the editorial staff are not received within **two months** of transmittal to the author, the submission will automatically be withdrawn. Should the manuscript require further revision, this would normally be expected to be completed within one month of the revision having been requested. 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 submitted the paper 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. Any change to the journal of publication will only be made after full discussion with the communicating author.

3.4. 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. The inclusion of material in an informal publication, *e.g.* a preprint server or a newsletter, does not preclude publication in an IUCr journal.

Important considerations related to publication have been given in the ethical guidelines published in *Acc. Chem. Res.* (2002), **35**, 74–76.

3.5. 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. Authors will be asked to transfer copyright during the electronic submission procedure.

3.6. 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.

3.7. Contact e-mail address

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

3.8. File format for accepted papers

The files required after acceptance of the paper are: a single file in WORD, RTF or LaTeX format of the text, tables and figure captions of the article; a high-resolution graphics file (minimum 600 d.p.i.) in TIFF, PostScript or encapsulated PostScript format for each figure and scheme; and files of any supplementary material not previously submitted.

3.9. File transfer for accepted papers

Files should be uploaded *via* the web at an address provided by the Co-editor. Full details of this procedure are given at **http://journals.iucr.org/s/services/submitbdy.html**.

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 §3.8.

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 §12.4)

5.1. Quality

Electronic files in the formats listed in §3.9 are essential for high-quality reproduction. The resolution of bitmap graphics should be a minimum of 600 d.p.i.

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; grids and shadings should be avoided where they are not required to improve clarity. Descriptive matter should be placed in the legend.

5.4. Numbering

Diagrams should be numbered in a single series in the order in which they are referred to in the text.

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. At the editor's discretion, figures printed in black and white may appear in colour in **Crystallography Journals Online**.

6. Tables

Authors submitting in Word should use the Word table editor to prepare tables.

6.1. Use of tables

Extensive 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.

Make sure only scalar variables and non-standard functions appear in italic font.

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 Commision 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.

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).

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.* B**45**, 383–390.
Ferguson, G., Schwan, A. L., Kalin, M. L. & Snelgrove, J. L. (1997). *Acta Cryst.* C**53**, IUC9700009.
Hervieu, M. & Raveau, B. (1983*a*). *Chem. Scr.* **22**, 117–122.
Hervieu, M. & Raveau, B. (1983*b*). *Chem. Scr.* **22**, 123–128.

International Union of Crystallography (2000). *(IUCr) Journal of Synchrotron Radiation*, http://journals.iucr.org/s/journalhomepage.html.
International Union of Crystallography (2001). *(IUCr) Structure Reports Online*, http://journals.iucr.org/e/journalhomepage.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.

11. Crystal structure determinations

Papers that report the results of crystal structure determinations of small molecules must report the associated experimental data as required in the Notes for Authors for *Section C* of *Acta Crystallographica*. These data should be supplied as a single electronic file in CIF format. The CIF will be checked in the Editorial Office in Chester for internal consistency.

12. Supplementary publication procedure (deposition)

12.1. 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 made available from the IUCr electronic archive *via* **Crystallography Journals Online** or to be deposited with the Protein Data Bank, the Nucleic Acid Database and the ICDD as appropriate.

12.2. 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; and

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.

12.3. Macromolecular structures

Authors should follow the deposition recommendations of the IUCr Commission on Biological Macromolecules [*Acta Cryst.* (2000). D**56**, 2]. 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.

12.4. Powder diffraction data

Authors of powder diffraction papers should consult the notes provided at **http://journals.iucr.org/services/cif/powder.html**.

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.

12.5. XAFS data

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

12.6. Other spectroscopic, diffraction and imaging data

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

13. Crystallography Journals Online

All IUCr journals are available on the web *via* **Crystallography Journals Online**; **http://journals.iucr.org/**. Full details of author services can be found at **http://journals.iucr.org/s/services/authorservices.html**.

13.1. Electronic status information

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

13.2. Proofs

Proofs will be provided in portable document format (pdf). The correspondence author will be notified by e-mail when the proofs are ready for downloading.

13.3. Open access

At the proof stage, authors will be given the opportunity to make their papers 'open access' on **Crystallography Journals Online**.

13.4. Reprints

After publication, the correspondence author will be able to download the electronic reprint of the published article, free of charge. Authors will also be able to order printed reprints at the proof stage.

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

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