Acta Crystallographica Section B
Structural Science
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Notes for Authors

1. Scientific scope of *Section B*

Section B of *Acta Crystallographica* publishes papers in which structure is the primary focus of the work reported. The central themes of *Section B* are the acquisition of structural knowledge from novel experimental observations or from existing data, the correlation of structural knowledge with physico-chemical and other properties, and the application of this knowledge to solve problems in the structural domain. *Section B* has broad chemical coverage, encompassing metals and alloys, inorganics and minerals, metal-organics and purely organic compounds. Biological, particularly macromolecular, structural science is now covered by *Section D*. A more complete definition of scientific scope is given in an Editorial [*Acta Cryst.* (1994), B**50**, 1–3].

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 15 journal pages (about 15 000 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. In *Section B*, it is unlikely that reports of individual structure determinations will be acceptable as *Short Communications*, since *Section C* of *Acta Crystallographica* exists for this purpose.

Short Communications should not exceed two journal pages (about 1500 words). A maximum of two figures and two tables of appropriate size are permitted.

All *Short Communications* should be submitted to the **Section Editor**.

2.3. Lead Articles

Lead Articles are authoritative, comprehensive and forward-looking reviews of major areas of research interest. They are always **commissioned by the Section Editor**, on the advice of the Editorial Board. Suggestions for suitable topics and of potential author(s) are welcomed by the **Section Editor** for discussion with the Board.

The Editor will discuss the treatment of the topic, the length of the *Article* and the delivery date of the manuscript with invited author(s). *Lead Articles* will be refereed in the normal manner.

2.4. Topical Reviews

A *Topical Review* is a short, highly focused survey covering a relatively narrow area of current research interest. It should not aim to be comprehensive, but a brief introduction should provide historical perspective and a brief conclusion should indicate likely future directions.

Topical Reviews will be limited to about ten journal pages (10 000 words) except in special agreed circumstances. Shorter reviews on rapidly evolving areas are also actively encouraged. They will be **commissioned by the Section Editor** either personally, **or following a formal proposal by prospective author(s)**. *Topical Reviews* will be refereed in the normal way.

2.5. Letters to the Editor

These may deal with non-technical aspects of crystallography, its role, its propagation, the proper function of its Societies *etc.*, or may make a technical observation or scientific comment that would usefully be brought to a wider audience. Letters should be submitted to the Section Editor or to the Editor-in-Chief of *Acta Crystallographica* only.

2.6. Scientific comment

Comments of general scientific interest to the readership are welcomed. These should not normally exceed two journal pages and should be submitted as in §3.

2.7. Meeting Reports

These are normally invited. Prospective authors interested in writing such items should first contact the Section Editor.

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.

2.9. Obituaries

These will be commissioned by the Section Editor.

3. Submission and handling of manuscripts

Papers should be submitted in one of two ways: either as hard copy directly to an editor **or** electronically *via* the web at http://journals.iucr.org/services/submit.html.

3.1. Hard-copy submission

Manuscripts and figures should be prepared using the file formats listed in §3.8. 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. Crystal data should be submitted in CIF format (see §11). Unless stated otherwise in §2, the submission should be sent to the Section Editor or any of the Co-editors. 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/b/services/editors.html**.

3.2. Electronic submission

Manuscripts and figures should be prepared using the file formats listed in §3.9. Full details of the submission procedure can be found at **http://journals.iucr.org/services/submit.html** and authors should first check this page to see if the service is available.

3.3. Languages of publication

Acta Crystallographica Section B will publish papers in English, French, German and Russian.

3.4. Handling of manuscripts

All contributions will be seen by referees (normally two) before they can be accepted for publication. The 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 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 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 a section of *Acta Crystallographica* other than that specified by the author(s), to the *Journal of Applied Crystallography* or to the *Journal of Synchrotron Radiation*. Any change to the section or 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 acknowledegments, 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. During the electronic submission process, authors will be asked to transfer copyright electronically.

3.7. Author grievance procedure

An author who believes that a paper has been unjustifiably treated by the Co-editor may appeal initially to the Section Editor and then to the Editor-in-Chief if still aggrieved by the decision.

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

The manuscript should be prepared using TEX, LATEX 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 should be provided in PostScript, encapsulated PostScript or TIFF formats. The resolution of bitmap graphics should be a minimum of 600 d.p.i.

3.10. File transfer

For electronic submissions the files should be uploaded *via* the web. Full details of this procedure are given at **http://journals.iucr.org/services/submit.html**.

For hard-copy submissions, final electronic files must have a filename constructed from the *reference number* supplied by the Co-editor. Files should be given the extensions `.tex`, `.doc` and `.rtf` as appropriate. Illustrations should be given the extensions `.ps`, `.eps` or `.tif`. Multiple files for the same submission should be uniquely identified, *e.g.* `xz1087fig1.ps`, `xz1087fig2.ps`, `xz1087.doc` *etc.*, where `xz1087` is the *reference number*.

Only after acceptance of the paper by the responsible editor should the final electronic version of the paper be sent to the Editorial Office in Chester. This may be *via* the web (see above), by e-mail (med@iucr.org), on diskette or by ftp as described below.

(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/b**
(v) Transfer a file from your account (*e.g.* j29.ps) as an identifiable name (*e.g.* ja0325fig1.ps):	**put j29.ps ja0325fig1.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 (**bpub@iucr.org**) with a list of the files transferred by ftp.	

4. Abstract and synopsis

All 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 as specifically and as quantitatively as possible 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. *Abstracts* should not exceed 200 words for *Abstracts* of *Research Papers*, *Lead Articles* and *Topical Reviews*, and 100 words for shorter contributions. Similarly, the title of the paer should be kept to a minimum length. It should make no reference to tables, diagrams, atom numbers or formulae contained in the paper. It should not contain footnotes. Numerical information given in the *Abstract* should not be repeated in the text. Crystal data should not be repeated in the *Abstract*. 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.* [Filippini (1990). *Acta Cryst.* B**46**, 643–645].

5. Diagrams and photographs ('figures')

Figures should be prepared using one of the file formats listed in §3.9.

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 papers reporting novel organic or metal-organic structures, it is mandatory that a chemical structural diagram be included for each compound.

In a charge-density 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 §12.3).

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 1200 d.p.i. Where electronic files are not available, 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.

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. Stereofigures

Atom labelling when included should be on both left and right views in stereo perspective. Both views should be incorporated into a single figure.

5.6. 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. Economy in use of tables

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

Structure factors, anisotropic displacement parameters, least-squares planes and unrefined H-atom coordinates are usually deposited as electronic files, see §11.

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 (×) 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 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.

Space groups should be designated by the Hermann–Mauguin symbols. Standard cell settings, as listed in **Volume A** of *International Tables for Crystallography*, should be used unless objective reasons to the contrary are stated. When a non-standard setting is used, the list of equivalent positions should be given. Hermann–Mauguin symbols should also be used for designating point groups and molecular symmetry. It is helpful if the origin used is stated explicitly where there is a choice.

The choice of axes should normally follow the recommendations of the Commission on Crystallographic Data [Kennard *et al.* (1967). *Acta Cryst.* **22**, 445–449].

A symbol such as 123 or *hkl* without brackets is understood to be a reflection, (123) or (*hkl*) a plane or set of planes, [123] or [*uvw*] a direction, {*hkl*} a form and ⟨*uvw*⟩ all crystallographically equivalent directions of the type [*uvw*]. Other bracket notations should be explicitly defined.

9.2. Nomenclature of chemical compounds *etc*.

Names of chemical compounds and minerals are not always unambiguous. Authors should therefore quote the chemical formulae, including chemical structural diagrams for organic and metal-organic compounds, 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 non-systematic name may be retained, but the corresponding systematic (IUPAC) name should also be given.

For crystal structures containing chiral molecules, authors should make it clear whether the crystal structure is a racemate or enantiopure, and if enantiopure whether or not the assignment of the absolute configuration is justified. For preference, absolute configuration should be indicated using the CIF data item _chemical_absolute_configuration. The title, compound

name, chemical diagrams, atomic coordinates and space group must correspond to the enantio-composition and the selected configuration. It is also most helpful to indicate the crystallographic and non-crystallographic symmetry of each molecule in the asymmetric unit.

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 following style:

Andrews, M., Wright, H. & Clarke, S. A. (2000). In preparation.

Bricogne, G. (1993). *Acta Cryst.* D**49**, 37–60.

Carter, C. W. Jr (1990). *Methods: a Companion to Methods in Enzymology*, Vol. 1, pp. 12–24. New York: Academic Press.

Collaborative Computational Project, Number 4 (1994). *Acta Cryst.* D**50**, 760–763.

Crowther, R. A. (1972). *The Molecular Replacement Method*, edited by M. G. Rossmann, pp. 173–178. New York: Gordon and Breach.

International Union of Crystallography (2000). *(IUCr) Crystallography Journals Online*, http://journals.iucr.org.

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

Jancarik, J. & Kim, S.-H. (1991). *J. Appl. Chem.* **24**, 409–411.

Olsnes, S. & Pihl, A. (1982). *Molecular Action of Toxins and Viruses*, edited by P. Cohen & S. Van Heyningen, pp. 51–105. New York: Elsevier.

Stanlow, D. J. (2000). *Acta Cryst.* B**56**. In the press.

Strong, R. K. (1990). PhD thesis, Harvard University, USA.

Vogel, A. (1978). *Textbook of Practival Organic Chemistry*, 4th ed. London: Longman.

Wang, B.-C. (1985). *Methods Enzymol.* **115**, 90–112.

Yariv, J. (1983). Personal communication.

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

Identification of individual structures in the paper by the use of database reference (identification) codes should be accompanied by a full citation of the original literature in the reference list. However, in tables containing more than ten such reference codes, citation in the reference list is not required.

11. Crystal structure determinations

Papers which 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 Crystallogaphica*. These data should be supplied as an electronic file in CIF format. Authors are asked to pre-check their CIF using checkCIF before submission by e-mailing the CIF to **checkcif@iucr.org**

Authors submitting their paper in hard-copy format (see §3.1) will be assigned a Co-editor code by the handling Co-editor. They will then be asked to upload their CIF at the address **http:/journals.iucr.org/services/submit.html**. Authors submitting their paper electronically (see §3.2) will be asked to upload their CIF during the submission process.

All numerical data in the CIF will be automatically checked using checkCIF, and duplication checks will be carried out against the relevant database. A review document, including these reports and a preprint of the *Experimental details* table, will be forwarded to the Co-editor, together with the CIF.

Each published paper will include a standard *Experimental details* table generated from the CIF. All other tabular data except the coordinates should be submitted as part of the manuscript; these data will not be checked against the CIF, as the CIF data are assumed to be the definitive archive. The coordinates will only be available in CIF format from **Crystallography Journals Online**; they will not generally be printed as a numbered table and should not be included in this form in submission.

Authors submitting incommensurate modulated structures should see the check-list given by Chapuis *et al.* [*Acta Cryst.* (1997), A**53**, 95–100].

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 deposited with the IUCr electronic archive, 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;

additional diagrams,

should be supplied in one of the formats given in §3.8.

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

12.3. Powder diffraction data

Authors of powder diffraction papers should consult the notes provided at the online CIF help page (http://journals.iucr.org/c/services/cifhelp.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.

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

13.3. 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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