Acta Cryst. (1993). B49, 1-5

International Union of Crystallography

Acta Crystallographica - Sections A and B
Notes for Authors

1. Submission

1.1. *Selection of journal*

Section A of *Acta Crystallographica* publishes papers reporting fundamental advances in all areas of crystallography. Section B publishes structurally based papers from disciplines throughout the natural sciences.

Papers will be considered for inclusion if they are of importance for the area to which they contribute and are written with clarity and logic of presentation.

1.2. *Languages and submission of manuscripts*

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

Every issue of each journal contains the names and addresses of the editors (Editor and Co-editors) and the Technical Editor. Manuscripts for Sections A and B of *Acta Crystallographica* may be submitted to any of the editors, but not to the Technical Editor.

Contributions should be submitted **in triplicate** to the editor most convenient for the author. This will normally be the nearest editor but contributions in French, German or Russian should preferably be submitted to an editor in the appropriate country.

The author should retain a copy of the manuscript for checking proofs.

1.3. *Machine-readable submissions*

Authors who have used TEX, LATEX, Wordperfect or Word to prepare their manuscripts are invited to send a machine-readable version with their submission. The following formats may be used: 3.5 and 5.25″ IBM-compatible, 3.5″ Apple Macintosh and 3.5″ Sun OS diskettes; 0.5″ 1600/6250 bpi magnetic tape.

1.4. *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 proper credit is given to others, that the manuscript has not been published (in any language), and that it is not being considered and will not be offered elsewhere while under consideration for an IUCr journal. For this reason, the submission must be made over the signature of at least one author.

1.5. *Copyright*

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

1.6. *Handling*

The editor to whom a paper is submitted is responsible for choosing referees and for accepting or rejecting the paper, including deciding its final form for publication and interpreting these Notes, when necessary.

If the paper is accepted, it is the responsibility of the Technical Editor to prepare the paper for printing; he may have to correspond with authors and/or the editor involved in order to resolve ambiguities or to obtain satisfactory figures or tables. The date of acceptance that will appear on the published paper will be the date on which the Technical Editor receives the last item needed.

1.7. *Author grievance procedure*

An author who believes his paper has been unjustifiably rejected by the Co-editor may appeal initially to the Editor for a new review and, finally, to the Editor of *Journal of Applied Crystallography* if the author is still aggrieved by the decision.

2. Categories of contributions

2.1. *Full articles*

All papers are sent to referees (ordinarily two) before they are accepted for publication. 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).

2.2. *Short Communications*

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.

Short Communications are not intended for interim reports of work in progress. Although such accounts may be accepted when they concern long-range projects, authors are requested not to submit them when completion of the work may reasonably be expected within eighteen months.

2.3. *Fast Communications*

Fast Communications should not normally exceed the equivalent of about 2000 words (or eight pages of double-spaced typescript). Figures should be clearly lettered. If the paper is available on diskette it would be helpful if this could be sent with the manuscript, together with details of the word-processing package used; it would also be helpful if complicated tables could be submitted as camera-ready copy. *Fast Communications* will be refereed promptly and prepared as camera-ready copy in Chester. 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, if the author so wishes.

2.4. *Letters to the Editor*

These may deal with non-technical aspects of crystallography, 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. *Letters* should be sent to the Editor only. They will not be refereed.

2.5. *Reviews*

The Commission on Journals occasionally invites leaders in selected areas to write Lead Articles, which are forward-looking reviews of specific topics. In addition, unsolicited review articles

may be submitted for publication in *Acta Crystallographica* or the *Journal of Applied Crystallography* by first submitting a brief outline of the proposed article for approval by the Editor. All selected Lead Articles and review articles will be refereed in the usual manner.

3. 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 the journal.

3.1. *Type style*

The editorial staff in Chester will indicate to the printer the style of type to be used. It is better that authors should not indicate type style at all rather than do so in a way different from that used by the printers. However, it is helpful if authors indicate vectors and tensors by a wavy underline.

3.2. *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 to use another type face if that indicated by the author is not readily available.

4. Abstract

All contributions must be preceded by an *Abstract* in English. 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. Ordinarily 200 words suffice for a full article and 100 words for shorter contributions. 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. 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')

5.1. *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 structural papers it is preferred that (i) distances and angles be given in tabular form and (ii) that a chemical structural diagram be included for organic and metal-organic compounds.

Supplementary diagrams may be deposited (see §10.1).

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 §10.4)

5.2. *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.

5.3. *Colour figures*

Figures in colour are accepted **at no cost to the author** if the editor considers them essential for a clear understanding of the paper.

5.4. *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$\times$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 80 mm). Figures at greater than column width are allowed at editorial discretion.

5.5. *Stereofigures*

The recommended limit on stereofigures is one per structure; more than one per structure may be included if the editor and referees feel that this is necessary for understanding the paper. Authors are reminded that a non-stereoview (half a pair) is often an acceptable alternative. Stereoviews should ordinarily fit into a single column (80 mm wide), the centre-to-centre separation (after reduction to 80 mm width) should be in the range 40 to 55 mm and atom labelling should be included on both left and right views in stereo perspective.

5.6. *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 (80 mm) width.

Lettering should be kept to a minimum; distances, bond angles and torsion angles should be given as tables and descriptive matter should be placed in the legend.

On diagrams and figures, the author's own lettering ready for photographing is preferred; if necessary, lettering will be added by the printer if a photocopy showing the required lettering is supplied with an unlettered original.

5.7. *Numbering and legends*

Diagrams and photographs are to 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. 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.

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

Structure factors, anisotropic displacement parameters, least-squares planes and unrefined H-atom coordinates are deposited, **except when the nature of the paper requires that they be immediately available.**

6.2. *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.

7. Nomenclature

7.1. *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.

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, Speakman & Donnay (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.

For the nomenclature of crystal families, Bravais-lattice types and arithmetic classes see de Wolff *et al.* [*Acta Cryst.* (1985), A**41**, 278–280].

For the nomenclature of polytypes see Guinier *et al.* [*Acta Cryst.* (1984), A**40**, 399–404].

For the nomenclature of inorganic structure types see Lima-de-Faria *et al.* [*Acta Cryst.* (1990), A**46**, 1–11].

For symbols for symmetry elements and symmetry operations see P. M. de Wolff *et al.* [*Acta Cryst.* (1992), A**48**, 727–732].

7.2. *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 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.

7.3. *Units*

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

8. References

References to published work must be indicated by giving the authors' names followed immediately by the year of publication, *e.g.* Neder, Frey & Schulz (1990) or (Neder, Frey & Schulz, 1990). Where there are six or more authors the reference in the text should be indicated in the form Smith *et al.* (1989) or (Smith *et al.*, 1989) *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.* and *J. Appl. Cryst.* are exceptions)], books, multi-author books, computer programs, personal communications and undated documents should be arranged alphabetically and conform with the following style:

Bürgi, H.-B. (1989). Acta Cryst. B45, 383–390.
Hervieu, M. & Raveau, B. (1983a). Chem. Scr. 22, 117–122.
Hervieu, M. & Raveau, B. (1983b). Chem. Scr. 22, 123–128.
Hummel, W., Hauser, J. & Bürgi, H.-B. (1990). In preparation.
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. Univ. of London, England.
Sheldrick, G. M. (1976). SHELX76. Program for crystal structure determination. Univ. 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.

9. Crystal structure determinations

Papers which report the results of crystal structure determinations of small molecules will have the associated numerical data checked in Chester for internal consistency. Such papers must comply with the requirements given in the Notes for Authors for Section C of *Acta Crystallographica*

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 British Library Document Supply Centre, with the Brookhaven Protein Data Bank and the ICDD as appropriate.

The information to be deposited is **at the discretion of the editor** and 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.

and for papers reporting results of crystal structure determinations:

Structure factors, weak reflections classified as unobserved should be included.

Anisotropic displacement parameters, including e.s.d.'s.

Least-squares planes and deviations from them.

Calculated H-atom coordinates.

Normal intermolecular distances.

Tables of non-essential bond lengths and angles (*e.g.* distances and angles in peripheral phenyl rings) or those of limited accuracy (*e.g.* those involving H atoms whose parameters have not been refined).

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*

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.

10.3. *Macromolecular structures*

If the structure determination is of a macromolecule, defined as any substance containing a polypeptide, polynucleotide or polysaccharide chain longer than 25 residues, deposition of atomic coordinates and structure factors is in machine-readable form with the Brookhaven Protein Data Bank.

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.

A paper concerned with a new technique for solving or refining structures is exempt from the deposition requirement if it does not report new structural information.

For the policy on publication and deposition of data from crystallographic studies of biological macromolecules see *Acta Cryst.* (1989), **A45**, 658.

10.4. *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 powder diffraction data (reported either in the paper or in the deposited material) to the International Centre for Diffraction Data (ICDD), 1601 Park Lane, Swarthmore, PA 19081-2389, USA. These data will then be checked and assigned an ICDD reference number which will, where possible, be published in the paper.

International Union of Crystallography

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