

Notes for authors

1. Scientific scope

Section A of *Acta Crystallographica* publishes articles reporting advances in the theory and practice of all areas of crystallography and structural science in the widest sense. As well as traditional crystallography, this includes nanocrystals, metacrystals, amorphous materials, quasicrystals, synchrotron and XFEL studies, coherent scattering, diffraction imaging, time-resolved studies and the structure of strain and defects in materials.

The central themes are, on the one hand, experimental and theoretical studies of the properties and arrangements of atoms, ions and molecules in condensed matter, and, on the other, the theoretical and experimental aspects of the various methods to determine these properties and arrangements.

2. Categories of contributions

The journal comprises two sections: **Advances** and **Foundations**.

Articles that are likely to be of high impact and broad interest will be considered for the **Advances** section of the journal. They will benefit from rapid publication (normally 6–8 weeks from submission) and may be accompanied by a Scientific Commentary (see §2.6) written for a scientifically literate audience and a press release upon publication. Authors may request that their article is considered for the **Advances** section when they submit their article (see <http://journals.iucr.org/a/services/submit.html> for more details).

Contributions should conform to the general editorial style of the journal. Typical articles may be viewed by going to http://journals.iucr.org/a/sample_issue.html. Articles should be written with a wide scientific audience in mind.

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.

Short Communications should not normally exceed two journal pages (about 1500 words).

2.3. Lead Articles

Lead Articles are authoritative, comprehensive and forward-looking reviews of major areas of research interest. Suggestions for suitable topics and of potential author(s) are welcomed by the Section Editors.

The Section Editors will discuss the treatment of the topic, the length of the *Article* and the delivery date of the article with invited author(s).

2.4. Feature Articles

Feature Articles are focused surveys covering recent advances in an area of current research. A brief introduction should provide historical perspective and a brief conclusion should indicate likely future directions. Inclusion of relevant new results is appropriate.

Feature Articles will generally be about ten journal pages (10 000 words). Shorter articles on rapidly evolving areas are also actively encouraged.

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 Editors.

2.6. Scientific Commentaries

Scientific Commentaries discuss articles of particular importance for the readership of the journal. Suggestions for suitable topics and of potential author(s) are welcomed by the Section Editors.

3. Submission and handling of articles

3.1. Submission

Articles should be submitted at <http://journals.iucr.org/a/services/submit.html>. Full instructions for submitting an article and details of the files required are given at <http://journals.iucr.org/a/services/submitinstructions.html>. Authors are encouraged to use the templates available from <http://journals.iucr.org/a/services/helpsubmit.html>. If the article reports a crystal structure, a CIF should be supplied (<http://journals.iucr.org/a/services/cifinfo.html>).

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

3.2. File format

The source files required for an article are: a single file in Word, OpenOffice or L^AT_EX format of the text, tables and figure captions of the article; a high-resolution graphics file (minimum 600 d.p.i.) in TIFF, PostScript, encapsulated PostScript or PNG format for each figure and scheme; and files of any supporting information. These should be uploaded as described in the **online submission instructions**.

3.3. Handling of articles

Advances articles will be seen by the Section Editors before peer review.

Each article is handled by an editor chosen by the author from a list of those available at the time of submission. Authors should choose an editor whose area of expertise most closely matches the subject of the article. Details of the current Editorial Board can be found at <http://journals.iucr.org/a/services/editors.html>.

All contributions will be seen by referees (normally two) before they can be accepted for publication. The editor to whom the article is assigned is responsible for choosing referees and for accepting or rejecting the article. This responsibility includes decisions on the final form of the article and interpretation of these Notes when necessary. Further information on the peer-review process can be found at <http://journals.iucr.org/a/services/peerreview.html>.

Changes to an article requested by the Section Editors, Co-editor or the editorial staff should be received within **two months** of transmittal to the author, otherwise the submission will be considered as withdrawn. If an article is not acceptable after two revisions it will not be considered further. Any subsequent communication of the material will be treated as a new submission in the editorial process. An article that has been rejected must not be resubmitted to any IUCr journal unless the reasons given for the rejection have been fully addressed in the revised version.

After initial submission, any revised or new files should be uploaded at the web address provided **only** in response to a specific request from an editor.

For accepted articles, it is the responsibility of the Managing Editor to prepare the article for publication. 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 article is the date on which the Managing Editor receives the last item required. Contact details for the Managing Editor of *Section A* can be found at <http://journals.iucr.org/services/contactus.html>.

On rare occasions, an editor may consider that an article is better suited to another IUCr journal. Any change to the journal of publication will only be made after full discussion with the contact author.

Articles will be checked for plagiarism using the CrossCheck service.

3.4. Author's warranty

The submission of an article is taken as an implicit guarantee that the work is original, that it is the author(s) own work, that all authors are aware of and concur with the submission, that all workers involved in the study are listed as authors or given proper credit in the acknowledgements, that the article 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.

The co-authors of an article should be all those persons who have made significant scientific contributions to the work reported, including the ideas and their execution, and who share responsibility and accountability for the results. Other contributions should be indicated in the acknowledgements. Changes to the list of authors will normally require the agreement of the editor and all authors.

The IUCr is a member of the Committee on Publication Ethics (COPE) and endorses its recommendations, including the Code of Conduct for Editors, which are available at <http://www.publicationethics.org/>. Important considerations related to publication have been given in the ethical guidelines published in *Acc. Chem. Res.* (2002), **35**, 74–76 and Graf *et al.* [*Int. J. Clin. Pract.* (2007), **61** (Suppl. 152), 1–26]. Authors are expected to comply with these guidelines.

3.5. Author grievance procedure

An author who believes that an article has been unjustifiably treated by the Co-editor may appeal initially to the Section Editors

for a new review and, finally, to the Editor-in-chief of IUCr Journals if the author is still aggrieved by the decision. The initial appeal must be made within three months of rejection of the article. The decision of the Editor-in-chief is final.

3.6. Copyright

Except as required otherwise by national laws, an author will be required to agree to the transfer of copyright before an article can be accepted. Authors selecting open access do not need to transfer copyright. Details of author rights can be found at <http://journals.iucr.org/services/authorrights.html>.

3.7. Open access

Authors are given the opportunity to make their articles 'open access' on **Crystallography Journals Online**. Authors of open-access articles will not be asked to transfer copyright to the IUCr, but will instead be asked to agree to an open-access licence. This licence is identical to the Creative Commons Attribution (CC-BY) Licence. Further details can be found at <http://journals.iucr.org/services/openaccess.html>.

3.8. Publication fees

There are no fees for colour figures or electronic reprints. If authors require open access or printed reprints there is a charge and details will be given at the proof stage.

4. Article preparation

4.1. General information

Before preparing articles, authors should consult a current issue of the journal to make themselves familiar with the general format, such as the use of headings, layout of tables and citation of references. A sample issue is available at http://journals.iucr.org/a/sample_issue.html.

All contributions must be accompanied by an English language *Abstract*, and a one or two sentence *Synopsis* of the main findings of the article for inclusion in the Table of Contents. Authors should also supply at least five keywords.

The *Abstract* should state as specifically and as quantitatively as possible the principal results obtained and their significance. For *Research Papers*, *Lead Articles* or *Feature Articles* the *Abstract* should be around 250 words. For shorter contributions 150 words should suffice. The *Abstract* should be suitable for reproduction by abstracting services without a change in wording and should not repeat information given in the title. It should make no reference to tables, diagrams, atom numbers or formulae contained in the article. It should not contain footnotes and should not include the use of 'we' or 'I'.

4.2. Quality of writing

Articles should be clearly written and grammatically correct. If the Co-editor concludes that language problems would place an undue burden on the referees, the article may be returned to the authors without review. Details of language-editing services can be found at <http://journals.iucr.org/services/languageervices.html>.

4.3. Diagrams and photographs ('figures')

A set of guidelines for preparing figures is available from <http://journals.iucr.org/a/services/help/artwork/guide.html>. Figures should be prepared using one of the file formats listed in §3.2.

The choice of figures should be optimized to produce the shortest article consistent with clarity. Duplicate presentation of the same information in both figures and tables is to be avoided, as is redundancy with the text. Supplementary figures may be deposited (see §5).

In articles which use powder-profile fitting or refinement (Rietveld) methods, figures that 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 §5.4).

4.3.1. Quality. Electronic files in the formats listed in §3.2 are essential for high-quality reproduction. The resolution of bitmap graphics should be a minimum of 600 d.p.i.

4.3.2. 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 (8.8 cm).

4.3.3. 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 for clarity. Descriptive matter should be placed in the caption.

4.3.4. Numbering and captions. Diagrams should be numbered in a single series in the order in which they are referred to in the text. A list of figure captions should be included in the article.

4.3.5. Colour figures. Colour figures are accepted at no cost to the author.

Authors preparing colour figures should consider how the figure would look if printed in greyscale and to readers who are colour-blind. It is very important that poor contrast (*e.g.* pale colours with a white background) be avoided.

4.3.6. Enhanced figures. An online tool for authors to prepare standard and corresponding three-dimensional interactive structural diagrams is available from <http://submission.iucr.org/jtkit>.

4.4. Tables

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

4.4.1. Use of tables. Extensive 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 §5.

4.4.2. 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.

4.5. Video and multimedia content

Multimedia content (*e.g.* time-lapse sequences, three-dimensional structures) is welcomed. For details of how to prepare enhanced three-dimensional figures, see §4.3.6. The preferred file formats for

multimedia are given at <http://journals.iucr.org/services/filetypes.html>.

4.6. 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.

Scalar variables and non-standard functions should appear in italic type.

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.

All displayed equations, including those in published Appendices, should be numbered in a single series.

4.7. Nomenclature

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

4.7.2. Crystallographic nomenclature. Authors should follow the general recommendations produced by the IUCr Commission on Crystallographic Nomenclature (see reports at <http://www.iucr.org/resources/commissions/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 *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 $\langle uvw \rangle$ all crystallographically equivalent directions of the type [*uvw*]. Other bracket notations should be explicitly defined.

4.7.3. 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 articles.

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 (IMA) 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.

4.8. 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.*

The reference list should be arranged alphabetically and conform with the following style:

- Chen, J. P. J., Spence, J. C. H. & Millane, R. P. (2014). *Acta Cryst.* **A70**, 143–153.
- Cowley, J. M. (1993). Editor. *Electron Diffraction Techniques*. Oxford University Press.
- CRC Handbook of Chemistry and Physics* (1983). 64th ed., edited by R. C. Weast, p. D-46. Boca Raton: CRC Press.
- Götz, D., Herres, N., Diehl, R. & Klapper, H. (2014). In preparation.
- Hudspeth, J. M., Goossens, D. J. & Welberry, T. R. (2014). *J. Appl. Cryst.* **47**, doi:10.1107/S1600576713034547.
- International Union of Crystallography (2014). (*IUCr*) *Crystallography Journals Online*, <http://journals.iucr.org/>.
- Keller, E. & Pierrard, J.-S. (1999). *SCHAKAL99*. University of Freiburg, Germany.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Shmueli, U. & Weiss, G. H. (1985). *Structure and Statistics in Crystallography*, edited by A. J. C. Wilson, pp. 53–66. Guilderland: Academic Press.
- Smith, J. M. (2004). Personal communication.
- Zhou, P. F. (1993). PhD thesis, McMaster University, Hamilton, Ontario, Canada.

Note that all authors and **inclusive** page numbers must be given.

Identification of individual structures in the article by use of database reference (identification) codes should be accompanied by a full citation of the original literature in the reference list.

Citations in supporting information should also appear in the main body of the article or be given in a related-literature section.

4.9. Crystal structure determinations

Authors of articles that report the results of crystal structure determinations of small molecules or materials must supply data as a single electronic file in CIF format. Structure-factor data in CIF format are also required.

5. Supporting information

5.1. Purpose and scope

Supporting information (such as experimental data, additional figures and multimedia content) that may be of use or interest to some readers but does not form part of the article itself will be made available from the IUCr archive. Arrangements have also been made for such information to be deposited, where appropriate, with other relevant databases.

5.2. IUCr archive

All material for deposition in the IUCr archive should be supplied in one of the formats described at <http://journals.iucr.org/services/filetypes.html>. Structural information (for small-molecule structures) should be supplied in CIF format.

5.3. Macromolecular structures

Authors should follow the deposition recommendations of the IUCr Commission on Biological Macromolecules [*Acta Cryst.* (2000), **D56**, 2]. For all structural studies of macromolecules, coordinates and the related experimental data (structure-factor amplitudes/intensities and/or NMR restraints) must be deposited at a member site of the Worldwide Protein Data Bank (<http://www.wwpdb.org/>) if a total molecular structure has been reported. Authors are encouraged to deposit their data with the wwPDB in advance of submission to the journal and to provide an mmCIF and a wwPDB validation report on submission. Authors must supply the wwPDB reference codes before the article can be published and the data must be released upon publication.

Authors are encouraged to make arrangements for the diffraction data images for their structure to be archived and available on request.

5.4. Powder diffraction data

Authors of powder diffraction articles should consult the notes provided at <http://journals.iucr.org/services/cif/powder.html>. For articles 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, should be deposited.

6. Author information and services

An author services page is available at <http://journals.iucr.org/a/services/authorservices.html>.

6.1. Author tools

A number of tools are available to help with the preparation of articles.

Word, OpenOffice and L^AT_EX templates can be downloaded from the author services page.

Table tools within the Word template, the table converter at <http://publicif.iucr.org/services/tools> or the program *publicIF* may be used to prepare tables of experimental details and geometric parameters suitable for inclusion in an article.

A toolkit for preparing enhanced figures is available at <http://submission.iucr.org/jtkf>.

For structural articles, CIFs can be checked using the *checkCIF/PLATON* service at <http://checkcif.iucr.org> and edited using *publicIF*, available from <http://publicif.iucr.org>.

6.2. Status information

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

6.3. Proofs

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

6.4. Reprints

After publication, the contact 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.

6.5. Open-access articles

The final published version of each open-access article is deposited with PubMed Central on behalf of the authors.

6.6. Publicising your article

There are many ways in which the IUCr promotes and raises awareness of articles published in its journals. More information on this and suggestions for how to publicise your articles can be found at <http://journals.iucr.org/a/services/articlepublicity.html>.

6.7. Crystallography Journals Online

All IUCr journals are available on the web *via* **Crystallography Journals Online** at <http://journals.iucr.org/>.