

## Notes for authors

### 1. Scientific scope

*Acta Crystallographica Section B* publishes scientific articles related to the structural science of compounds and materials in the widest sense. Knowledge of the arrangements of atoms, including their temporal variations and dependencies on parameters such as temperature and pressure, is often the key to understanding physical and chemical phenomena and is crucial for the design of new materials and supramolecular devices. *Acta Crystallographica Section B* is the forum for the publication of such contributions. The journal publishes scientific developments based on experimental studies as well as those based on theoretical approaches, including crystal-structure prediction, structure–property relations and the use of databases of crystal structures.

Scientific developments related to X-ray, electron and neutron diffraction studies of periodic and aperiodic crystals, fully and partially ordered solids as well as amorphous solids, clusters and single molecules are reported. Studies based on complementary techniques, like electron microscopy and other imaging or spectroscopic techniques, are also welcome. The journal covers inorganic, organic, organometallic and metal-organic compounds, minerals, metals, and alloys, as well as extended framework structures, and hybrid and biomimetic materials. A full list of topics can be found on the journal home page at <http://journals.iucr.org/b/journalhomepage.html>.

### 2. Categories of contributions

Contributions should conform to the general editorial style of the journal. Typical articles can be viewed by going to [http://journals.iucr.org/b/sample\\_issue.html](http://journals.iucr.org/b/sample_issue.html).

#### 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 for discussion with the Board.

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

### 2.4. Feature Articles

*Feature Articles* are focused surveys covering recent advances in an area of current research. They should not aim to be comprehensive, but 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. Research Perspectives

*Research Perspectives* are articles invited by the Section Editors after discussion with the Board. The main or sole author will be an established leader in a particular field and such articles are expected to review the development of that field, with a strong focus on the author's own contributions to it.

The length of a *Research Perspective* should not normally exceed 15 journal pages (about 15 000 words), but the Section Editors will discuss the length, the treatment of the topic and the delivery date of the manuscript with the invited author. The journal will normally publish one article in this category per year.

### 2.6. 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.

### 2.7. 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.

### 2.8. Special issues

*Acta Crystallographica Section B* also publishes focused special issues on topics which highlight the scope of the journal. For more information contact the Section Editors.

## 3. Submission and handling of articles

### 3.1. Submission

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

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

## 3.2. File format

The source files required for an article are: a single file in WORD, OpenOffice, L<sup>A</sup>T<sub>E</sub>X or CIF 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 (see §6.2). Files should be uploaded as described in the **online submission instructions**.

## 3.3. Handling of articles

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/b/services/editors.html>.

Firm positive recommendations from two independent referees are required before a submission 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/b/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 **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 B* can be found at <http://journals.iucr.org/b/services/contactus.html>.

On rare occasions, an editor may consider that an article is better suited to another IUCr journal. Any change to the section or 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 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.

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 COPE (Committee on Publication Ethics) 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 3 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 a manuscript 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/b/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/b/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/b/sample\\_issue.html](http://journals.iucr.org/b/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/languageservices.html>.

#### 4.3. Diagrams and photographs ('figures')

A set of guidelines for preparing figures is available from <http://journals.iucr.org/b/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 §6).

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 §6.3).

**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 to improve 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 manuscript.

**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 in greyscale and to readers who are colour-blind. It is important that poor contrast (*e.g.* pale colours with a white background) be avoided.

**4.3.6. Chemical line diagrams and schemes.** In articles reporting organic or metal-organic structures, a chemical line diagram should normally be included for each compound. The diagram should be complete, showing all species present in the structure, including counter-ions and solvent molecules in their correct proportions. Structures should be numbered (I), (II), (III) *etc.*

Chemical line diagrams and reaction schemes should not have a caption.

Authors are encouraged to submit chemical connectivity (MOL, CML, CHM, SMI) files of reported structures with their articles. These can often be generated by the software used to generate the

scheme. These files will be made available as part of the supporting information for each article and will be used to provide InChI (International Chemical Identifier) keys for the article, making the structures easier to find in the chemical literature.

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

#### 4.4. Tables

For single-crystal, powder, and modulated and composite structures, a standard experimental table (see §5) must be included. This table should be prepared using the table tools within the Word template (available from <http://journals.iucr.org/services/docx-template/>) or the table tool at <http://pubcif.iucr.org/services/tools>. These tools can also be used to create geometry tables.

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

Atomic coordinates and displacement parameters must be included in the CIF and are not normally repeated in the article. Derived values of only routine interest should be included in the CIF only. Structure factors should be deposited electronically; note that if structure factors are embedded in the CIF, separate structure factor files are not required.

**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 §4.3.7. 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. 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.

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 supported by experimental evidence. The 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.

**4.7.3. Crystallographic nomenclature.** Authors should follow the general recommendations produced by the IUCr Commission on Crystallographic Nomenclature (see reports at <http://www.iucr.org/iucr/commissions/cnom.html>).

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.

## 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:

- Allen, F. H. (2002). *Acta Cryst.* **B58**, 380–388.  
 Andrews, M., Wright, H. & Clarke, S. A. (2013). In preparation.  
 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.* **D50**, 760–763.  
 Crowther, R. A. (1972). *The Molecular Replacement Method*, edited by M. G. Rossmann, pp. 173–178. New York: Gordon and Breach.  
 Gavezzotti, A. (2010). *Acta Cryst.* **B66**, doi:10.1107/S0108768110008074.  
 Hervieu, M. & Raveau, B. (1983a). *Chem. Scr.* **22**, 117–122.  
 Hervieu, M. & Raveau, B. (1983b). *Chem. Scr.* **22**, 123–128.  
 International Union of Crystallography (2009). (*IUCr*) *Structure Reports Online*, <http://journals.iucr.org/e/journalhomepage.html>.  
 Jancarik, J. & Kim, S.-H. (1991). *J. Appl. Chem.* **24**, 409–411.  
 Kiser, P. D., Lodowski, D. T. & Palczewski, K. (2007). *Acta Cryst.* **F63**, doi:10.1107/S1744309107020295.  
 Ng, S. W. (2004). Private communication (refcode IXEQIL). CCDC, Cambridge, England.  
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
 Smith, D. (2010). *Acta Cryst.* **B66**. In the press.  
 Strong, R. K. (1990). PhD thesis, Harvard University, USA.  
 Vogel, A. (1978). *Textbook of Practical Organic Chemistry*, 4th ed. London: Longman.  
 Wang, B.-C. (1985). *Methods Enzymol.* **115**, 90–112.  
 Yariv, J. (1983). Personal communication.

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

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

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

## 5. Crystal structure determinations

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. Authors are asked to check their CIF with checkCIF before submission by using the checkCIF service at <http://journals.iucr.org/services/cif/checking/checkbasic.html>.

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 article will normally include a standard *Experimental details* table. Authors should use the table tools within the WORD template (available from <http://journals.iucr.org/services/docxtemplate/>), the table converter at <http://publif.iucr.org/services/tools/> or the program *publCIF* (available from <http://publif.iucr.org>) to generate this table from the CIF. The tools can be used to prepare the tables from CIFs for most kinds of studies (including determinations of modulated and composite structures from single-crystal and powder data). The table and all other tabular data except the coordinates should be submitted as part of the manuscript. If the number of structures reported is very large, if a single structure is reported as a function of temperature or composition, or if structures already in the literature have been redetermined, the author may request or the editor may require that an abbreviated table be prepared using the tools above. Atomic coordinates will be published

in CIF format only (see §6.2). Coordinates will only be included as a numbered table in very exceptional cases.

For articles reporting molecular structures a labelled displacement ellipsoid molecular diagram is normally required for publication; for non-molecular structures, a packing or polyhedron diagram may be more appropriate. If the number of structures reported is large it may be preferable to put some or all of the diagrams in the supporting information. Atomic displacement parameters for all structures reported will be available in the CIF during review and after publication. Any unusual features of these parameters should be either illustrated in a figure or mentioned in the article text.

Authors submitting incommensurate modulated structures should see the checklist given by Chapuis *et al.* [*Acta Cryst.* (1997), **A53**, 95–100].

## 6. Supporting information

### 6.1. 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.

### 6.2. 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.

### 6.3. 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, must be deposited.

## 7. Author information and services

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

### 7.1. Author tools

A number of tools are available to help with the preparation of articles. Word, OpenOffice and L<sup>A</sup>T<sub>E</sub>X templates can be downloaded from the author services page. Table tools with the WORD template, the table converter at <http://publicif.iucr.org/services/tools> or the program *pubCIF* 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/jtk>.

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

### 7.2. Status information

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

### 7.3. Proofs

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

### 7.4. 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.

### 7.5. Open-access articles

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

### 7.6. 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 on how to publicise your articles can be found at <http://journals.iucr.org/b/services/articlepublicity.html>.

### 7.7. Crystallography Journals Online

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