

Checklist for Authors of Papers Submitted to *Journal of Applied Crystallography*

The *Journal of Applied Crystallography* is concerned with methods, apparatus, problems and discoveries in applied crystallography. It is intended to meet the needs of those scientists in governmental, industrial, and university research laboratories who use crystallographic techniques, especially diffraction methods, to study materials and to control their quality.

Papers are accepted on such topics as the applications of crystallographic techniques to analytical problems, to metallurgy, to chemistry (with the exception of structure determinations), to solid state physics (degree of order, imperfections, etc.), to the determination of lattice parameters, crystallite size, strain, etc., to the study of crystalline orientation and texture, and to studies of fibrous, partly crystalline, amorphous, and liquid materials. Papers are welcome on instrumentation, experimental techniques, crystallographic aids, computer programs, specimen preparation, crystal growth, etc., and on crystallographic applications of other techniques (electron microscopy, electron microprobe, spectroscopy, etc.).

The checklist below is given for the convenience of authors submitting papers for publication in *Journal of Applied Crystallography*. These details have been extracted from *Notes for Authors* [*Acta Cryst.* (1983), **A39**, 174–186] to which authors are referred for full information. The attention of authors is also drawn to the *Suggested guidelines for the publication of Rietveld analyses and pattern decomposition studies* [*J. Appl. Cryst.* (1982), **15**, 357–359].

Occasionally Lead Articles are published in *Journal of Applied Crystallography*. Although these may contain a review element, their primary emphasis will be with the direction in which the subject is moving, indicating major problems, with suggestions for the future development of the subject. Lead Articles will normally be invited, but authors wishing to contribute such a paper are asked to discuss their proposal with the Editor in advance. Such articles will be subject to normal review.

Journal of Applied Crystallography also includes Short Communications and several categories of information. These are:

Crystal Data. Both powder data and single-crystal data of well characterized materials are accepted if they are of high quality and convey original information, although this section is not intended to include preliminary reports of structure determinations. Such data must be submitted in a prescribed format (see *Notes for Authors*, Appendix II). Only the Title, Abstract and acknowledgements are published; the remaining parts of these contributions are deposited.

Computer Programs. A brief description of the purpose, strategy, computer language, machine requirements, input requirements, and the type of results obtained

should be included. It is also ordinarily required that the adequacy of the documentation shall have been proven by the successful use of the program by someone outside the author's institution.

Computer Program Abstracts. This future section is intended to provide readers with information on new crystallographic computer programs, without giving the detail required in the *Computer Program* section. The information required is detailed below.

Laboratory Notes are very brief descriptions (further details being obtainable from the authors) of special devices, equipment modifications, techniques for accomplishing certain common tasks, etc. A simple schematic drawing may often be preferable to an actual photograph of apparatus. *Laboratory Notes* should be written in such a manner that the first sentences form an abstract of the whole Note.

Letters to the Editor 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.

Meeting Reports. These are normally invited.

Crystallographers. This category is intended to be a collection of short paragraphs dealing with the activities of crystallographers, such as their changes of position, promotions, assumption of significant new duties, honours, obituaries, etc. Contributions should be sent to the Executive Secretary of the Union.

New Commercial Products. Brief announcements of new commercial products, including prices and manufacturer, will be carried in future. Announcements should be sent to the Editor.

All papers submitted for publication in the *Journal of Applied Crystallography* should be checked against the following list:

- (a) Signed *Transfer of Copyright* form with manuscript
- (b) *Typescripts*
 - Submitted in triplicate to any Coeditor or the Editor
 - Double-spaced with wide margins (e.g. 30 mm)
 - Authors' addresses in full
 - Maximum of 10000 words for regular contributed papers
 - Maximum of 1000 words for Short Communications (For typography see *Notes for Authors*, §9)
- (c) *Title*
 - Short and informative
 - For *Crystal Data* see *Notes for Authors*, Appendix II
- (d) *Abstract*
 - About 200 words
 - Suitable for reproduction by abstracting services without change of wording

Principal results stated as specifically and quantitatively as possible

Sufficiently informative to obviate need for *Conclusion(s)* section

(e) *Experimental and computational details*

Sufficient information to permit calculations and measurements to be repeated or extended by others and allow independent evaluation of the results.

Details of all computer programs used

For *Computer Programs* and *Computer Program Abstracts* evidence that program has been successfully used by others

For *Computer Program Abstract* details see below

(f) *Mathematical derivations*

Abbreviated as far as is practicable without loss of clarity

Full mathematical derivations and mathematical appendices to be deposited

Symbols explained if not clear or commonly used

(g) *Diagrams and photographs*

Drawings in black ink or high-quality glossy prints

Cited in text

As small as possible consistent with legibility

High information density

Lettering not less than 4 mm on International A4 (210 × 297 mm) sized or 8½ × 11 in paper (and *pro rata*)

Figure captions in separate list

(h) *Tables*

Not to report information in text or diagrams

Cited in text

Table number and title for each

To occupy minimum space consistent with clarity

To include e.s.d.'s for all derived quantities (especially all varied parameters)

If very long, example should be given and complete table deposited

For *Crystal Data* see *Notes for Authors*, Appendices II and III

(i) *References*

In form: authors' names followed by year of publication

Alphabetic order in reference list

All references in text to be given in reference list and *vice-versa*

Inclusive page numbers to be given in reference list

(j) *Units and Nomenclature*

SI units to be used throughout (except for Å)

All acronyms to be defined

Atom labels as C(l) *etc.*

Space groups in Hermann–Mauguin notation (Schönflies symbols may be used in addition for molecular symmetry)

Choice of axes as recommended by Kennard, Speakmann & Donnay [*Acta Cryst.* (1967), **22**, 445–449]

Symmetry-equivalent atoms to be denoted as C(1ⁱ) *etc.*

Reflections, planes, directions and forms to be unambiguously distinguished (see *Notes for Authors*, §8)

Chemical names and formulae to conform to IUPAC rules, including spelling of element names

Nomenclature of polytypes to conform to Guinier recommendations [*Acta Cryst.* (1984), **A40**, 399–404]

(k) *Data to be deposited*

In general:

Complete *Crystal Data* contributions (Title, Abstract and acknowledgements also printed; powder data also sent to JCPDS — see *Notes for Authors*, Appendices II, III)

At the Co-editor's discretion:

Details of experimental procedure

Details of mathematical derivations

Lengthy mathematical appendices

Lengthy discussion not of general interest

Nonessential tables of which only examples are printed

Figures of which examples are printed or that duplicate information given elsewhere

Format of deposited material:

Not to exceed A4 size (210 × 297 mm) or 8½ × 11 in

Minimum character height 1.5 mm

Three copies, of good photocopyable quality

(l) *Requirements for Computer Program Abstracts*

Give

Title of program or set of programs

Authors and addresses

Description of program(s) in not more than 200 words

Software status

Hardware requirements

Documentation available

Text status

Availability and where from

Names of those, outside the authors' laboratory, who have used and tested the program(s) (to be given in letter of submission, not in abstract itself)