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International Union of Crystallography

Notes for Authors

Contents

1. Submission of contributions 174
   1.1 Selection of journal 174
   1.2 Languages and to whom to submit manuscripts (typescripts) 175
   1.3 Author's warranty 175
   1.4 Copyright 175
   1.5 Preparation and handling 175

2. Categories of contributions 175
   2.1 Full articles 175
   2.2 Short communications 175
   2.3 Other short contributions in *Journal of Applied Crystallography* 175

3. Typescripts 176
   3.1 Paper, margins, spacing, general style 176
   3.2 Poorly prepared typescripts 176
   3.3 Addresses; responsible author 176
   3.4 Number of copies 176
   3.5 Manuscript length 176

4. Title and abstract 176
   4.1 Title 176
   4.2 Abstract 176

5. Diagrams and photographs ('figures') 177
   5.1 Design 177
   5.2 Quality, backing, colour 177
   5.3 Size 177
   5.4 Stereofigures 177
   5.5 Lettering and symbols 177
   5.6 Numbering and legends 177

6. Tables 177
   6.1 Economy in use of tables 177
   6.2 Design and size 177

7. References 178

8. Nomenclature 178
   8.1 Crystallographic nomenclature 178
   8.2 Nomenclature of chemical compounds *etc.* and minerals 179
   8.3 Units 180
   8.4 Abbreviations 180

9. Typography 180
   9.1 Conventions for indicating type style 180
   9.2 Mathematics and letter symbols 180
   9.3 Chemical and structural formulae 180

10. Computational details 180

11. Supplementary publication procedure (deposition) . . 181
   11.1 Purpose and scope 181
   11.2 Deposition procedure 182
   11.3 Preparation of hard copy for deposit 182
   11.4 Procedure for obtaining copies of deposits . . . 182

Appendix I. Criteria for publication in *Acta Crystallographica*, Sections B and C, and format for papers to be published in Section C . . . 182

Appendix II. Format for 'Crystal Data' 183

Appendix III. Standards for the publication of powder profile fitting (Rietveld) analyses and of powder pattern data 184

Transfer of Copyright Agreement 186

Notes for Authors

1. Submission of contributions

1.1 *Selection of journal*

The International Union of Crystallography publishes two journals, *Acta Crystallographica* and *Journal of Applied Crystallography*. Between them they cover all branches of crystallography, including new crystallographic apparatus; papers in related fields (physics, chemistry, mineralogy, metallurgy, biology, mathematics) that have a structural basis or crystallographic application are also accepted.

Acta Crystallographica appears in three sections:

Section A – *Foundations of Crystallography*,
One Volume, six parts per year.

Section B – *Structural Science*;
One Volume, six parts per year.

Section C – *Crystal Structure Communications*;
One Volume, twelve parts per year.

Papers concerned with basic developments in any area of crystallography should be submitted to Section A, structurally based papers from disciplines throughout the natural sciences should be submitted to Section B, which is intended to provide a show-case for exciting papers on all aspects of structural science. Papers reporting crystal structure determinations should be submitted to Section C.

The *Journal of Applied Crystallography* is concerned with the application of crystallography and crystallographic techniques, other than crystal structure determination, and with the apparatus, techniques and other factors involved.

Both journals publish contributed articles, Short Communications and Book Reviews. In addition, the *Journal of*

Applied Crystallography publishes various other categories of papers, details of which are given in § 2.3. Occasional review papers are also invited by this journal.

1.2 *Languages and to whom to submit manuscripts (typescripts)*

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 may be submitted to any of the editors, but not to either the Technical Editor or to the Editor of *Acta Crystallographica*. Papers for *Acta Crystallographica* should be clearly marked as to the Section for which they are intended.

Contributions should be submitted 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.

1.3 *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 the author believes it to be of suitable scientific standard for an IUCr journal, 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. All subsequent correspondence on the manuscript will be with this author.

1.4 *Copyright*

Except as required otherwise by national laws, an author must sign and submit a copy of the Transfer of Copyright Agreement (found at the end of these Notes) for each manuscript before it can be accepted. An explanation of the need for written transfer of copyright has been given elsewhere [*Acta Cryst.* (1978), A**34**, 158; *J. Appl. Cryst.* (1978), **11**, 63].

1.5 *Preparation and 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 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.

Two useful publications on the preparation of papers are: *Writing Scientific Papers in English* by M. O'Connor & F. P. Woodford (1976, Amsterdam: Elsevier) and *How to Write and Publish a Scientific Paper* by R. A. Day (1979, Philadelphia: ISI Press).

Authors are requested to give particular attention to the details of preparation outlined in the following sections.

2. Categories of contributions

2.1 *Full articles*

Full articles on all aspects of crystallography are distributed between the sections of *Acta Crystallographica* and *Journal of Applied Crystallography* as described in § 1.1. All papers are sent to referees (ordinarily two) before they are accepted for publication.

Acta Crystallographica: Section A publishes papers reporting fundamental advances in all areas of crystallography; Section B welcomes structurally based papers from disciplines throughout the natural sciences; and Section C includes all papers concerned with the determination and refinement of crystal structures *per se*, such as were previously published in Section B and in *Crystal Structure Communications* (*CSC*) (see Appendix I). The overall format of papers in Section C will resemble that previously used for Short Structural Papers (SSP) but without a specific length restriction. Conciseness will remain an important criterion in their evaluation. The *Introduction* section, which in SSP's contained the experimental details, will be replaced by a new *Introduction* (analogous to the *Preliminary Information* in *CSC*) and an *Experimental* section, the latter giving the essential experimental information in tabular form or in an abbreviated telegraphic form similar to that used for the crystal data in the *Abstract*.

A typical Section C paper is likely to include (1) a table of atomic coordinates and isotropic or equivalent isotropic thermal parameters, (2) a table or figure giving intramolecular bond distances and angles (see §§ 5.1 and 6.1), (3) one figure showing a projection of the molecule with thermal ellipsoids and atomic numbering and (4) one figure showing the packing, either as a stereoview or as a projection. Most papers will be expected to conform to this 'typical' pattern, with additional tables and figures deposited as a Supplementary Publication. Papers on more than one material, or on materials at more than one temperature or pressure, may be appropriately scaled in content. All duplicated information (except *R*) within the paper will be deleted.

Details of the criteria for publication in Sections B and C and the format of papers for Section C are given in Appendix I.

2.2 *Short Communications*

Short Communications differ from ordinary articles not only in being shorter (see § 3.5), but also in being printed in smaller type and in being handled more quickly. 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. *Other short contributions in Journal of Applied Crystallography*

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 (Appendices II and III). Only the *Title*, *Abstract* and

acknowledgements are published; the remaining parts of these contributions are deposited under the Supplementary Publication Scheme (§ 11). Crystal Data are sent to referees in the normal way.

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 Programs are sent to referees in the normal way.

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.* These are, generally, the kind of thing one makes note of when visiting someone else's laboratory, but which ordinarily are considered 'too small' to warrant publication. 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. They may be sent to any editor of *Journal of Applied Crystallography.*

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.

Forthcoming Meetings and Short Courses gives details of meetings of scientific societies, congresses, summer schools, *etc.* of interest to crystallographers. The *Calendar of Events* summarises all previously published events. Contributions should be sent to the Executive Secretary of the Union.

Laboratory Notes, Letters to the Editor, Meeting Reports and Crystallographers are not refereed, and are distinguished by a different typeface and layout.

3. Typescripts

3.1 *Paper, margins, spacing, general style*

Contributions should be typed on one side only of good quality paper, should be double-spaced with wide margins (*e.g.* 30 mm), and should conform to the general editorial style of the journal. Clarity for the printer is essential; elegance, in itself, is not.

3.2 *Poorly prepared typescripts*

Badly prepared typescripts unavoidably suffer delay in publication. Typescripts which would involve much editorial work will be returned to the author to be brought to the standard that should reasonably be expected of his institution or circumstances, see § 1.5.

3.3 *Addresses; responsible author*

Each author's address should be given in sufficient detail to ensure that correspondence will reach him. Postal code (zip code, *Postleitzahl, code postal, почтовый индекс*) should be included. In the absence of other written instructions on or with the typescript all correspondence including the proofs and reprint order form will be sent to the first-named author at the address given in the heading of the paper.

3.4 *Number of copies*

Manuscripts (including all figures and tables and material for deposit) should be submitted in triplicate, as this speeds the refereeing process by permitting two referees to work at the same time. Additionally, authors should retain an exact copy of the manuscript for checking proofs, as the manuscript will not be returned with the proofs.

3.5 *Manuscript length*

Brevity of presentation is essential. Only exceptionally can papers be considered which exceed the equivalent of about 6000 words. Articles intended for publication as Short Communications should not exceed the equivalent of about 1000 words. The primary consideration, however, is the provision of maximum density of information consistent with clarity of presentation. Duplicate presentation of information should be avoided.

4. Title and abstract

4.1 *Title*

The *Title* should describe concisely the subject of the paper. Introductory phrases such as 'A contribution to the theory of ...' or 'The crystal and molecular' preceding 'structure' ... are ordinarily unnecessary. Titles of crystal structure papers must identify unambiguously the substance studied (see Appendix I and § 8.2).

4.2 *Abstract*

All full articles, Short Communications, Crystal Data and Computer Programs 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. Numerical information given in the *Abstract* should not be repeated in the text. It should not include the use of the pronouns '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.* [Borie (1982). *Acta Cryst.* A**38**, 248–252].

A format is prescribed for the *Abstracts* of papers in Section C of *Acta Crystallographica* in Appendix I. Where applicable, the *Abstracts* of papers in Section B of *Acta Crystallographica* should follow the same format.

For the *Abstracts* of Laboratory Notes see § 2.3; for those of Crystal Data see Appendix II.

The *Guide for the Preparation of Author's Abstracts for Publication*, published by UNESCO (reference SC/MD/5, p. 5), is accepted by the International Union of Crystallography as a basis for its *Abstracts*. Copies are provided by the Technical Editor on request.

5. Diagrams and photographs ('figures')

5.1 *Design*

The choice of tables and figures used 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. For example, in structural papers it is preferred that bond lengths and bond angles be indicated on a well-designed ball-and-stick or thermal ellipsoid plot, whenever this is without ambiguity and is reasonably compact; the corresponding table should then be omitted entirely or, if the author prefers, deposited. The use of a thermal-ellipsoid plot will also give an indication of any unusual anisotropy in the thermal-vibration ellipsoids. Neither a ball-and-stick figure nor a thermal-ellipsoid plot is a satisfactory substitute for an organic structural formula, unless it shows clearly the complete molecule.

Supplementary diagrams are acceptable for deposit under the auxiliary publication procedure (§ 11).

In a charge density paper only those figures (one or two) 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 ($I_{obs} - I_{calc}$). As primary diffraction data cannot be satisfactorily extracted from such figures, the basic diffraction data should be deposited (see § 11.1 and Appendix III).

5.2 *Quality, backing, colour*

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. Diagrams should not be submitted on fragile material.

If they meet the other requirements, good quality reduced photographic copies of large diagrams are more satisfactory than original drawings.

The general requirements stated below for diagrams apply also to photographs. Photographs intended for half-tone reproduction must be in the form of highly glazed unmounted prints. The author should indicate on a photocopy which features of the photograph he would like reproduced most faithfully. Plates in colour or black and white are accepted only if the entire cost is paid for by the author or his organization.

5.3 *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 × 297 mm). They will usually 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, except for Laboratory Notes, where the column width is 52 mm). See also § 5.5. Co-editors will need to be satisfied that the information density is high enough, if authors wish figures to be printed larger than this. Comparable diagrams should ordinarily be presented on the same scale.

5.4 *Stereofigures*

The limit on stereofigures is one per structure unless the Co-editor and referees feel that more are necessary for understanding the paper. Authors are reminded that a non-stereo view (half a pair) is often an acceptable alternative. Stereoviews must fit into a single column (80 mm wide) and at this size the relative sizes of the molecule and the whole figure should be such that the individual atoms are easily distinguishable. The centre-to-centre separation in stereofigures must not exceed 55 mm. Atom labelling should be included on both left and right views in stereo perspective.

5.5 *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. Subject to considerations in §§ 5.1 and 6.1, lettering should be kept to a minimum: descriptive matter should be placed in the legend rather than in the diagram.

On diagrams and figures, the authors' own lettering ready for photographing is preferred if it is of suitable size, is reasonably consistent with the style of the journals, and is securely fixed in place. Symbols denoting units (SI), when given on ordinate or abscissa scales, should be included in round brackets.

5.6 *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. Every figure must have a legend to be printed below it. A list of the legends ('figure captions') is to be attached to the manuscript.

6. Tables

6.1 *Economy in use of tables*

Although numerical information is generally most economically presented in tables, diagrammatic representation of bond lengths and bond angles is preferred on one figure when this is reasonably compact (see § 5.1). Text and diagrams should not be redundant with the tables. Small tables will normally be set in type while large tables either will be photographically reproduced or (more usually) deposited. Structure factors, anisotropic thermal parameters, least-squares planes and unrefined H-atom coordinates are deposited, except when the nature of the paper requires that they be immediately available (see §§ 10, 11).

6.2 *Design and size*

Tables must be numbered in a single series of arabic numerals and 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 typed in single spacing, without excessive space between columns.

7. References

References to published work must be indicated by giving the authors' names followed immediately by the year of publication in parentheses, as, for example, '(Smith, Jones & Robinson, 1982)', or 'Smith, Jones & Robinson (1982)'. Unpublished but dated documents may be referred to in the same way as publications. In the case of a document bearing no date the word 'undated' (*non daté, undatiert, Недатированный*) should be used instead of the year. If two or more separate references by exactly the same author or authors were published in the same year, they are distinguished by adding the letters, *a*, *b*, *etc.* to the dates. For private communications the year of communication should be stated. For documents which are in the course of publication but have not appeared the current year should be stated. Such publications should be described as 'in the press' (*sous presse, im Druck, в печати*) if they have reached the printers. Otherwise they should be described as 'in preparation' (*en preparation, in Vorbereitung, в предготовлений*) or as having been submitted to or accepted for publication by a particular journal. Dates and spellings of authors' names (including accents and diacritical marks) must be everywhere correct and consistent.

At the end of the paper a list giving full details of all references should be appended separately. The references should (i) be arranged in alphabetical order of authors' names, (ii) include the initials of all authors. Note that 'Smith, J. R. (1976)' precedes 'Smith, J. R. & Jones, T. D. (1970)'. Except for *Acta Cryst.* and *J. Appl. Cryst.*, names of Journals should be abbreviated in accordance with the *Bibliographic Guide for Editors and Authors* (1974), published by the American Chemical Society or with the *International List of Periodical Title Word Abbreviations* [ISO 833-1974(E)]; in cases of doubt the journal name should be given in full. References to books should give the full title, editors, volume and page numbers if necessary, place of publication, and name of publisher, in that order. Some examples of references to papers, books and other sources, as properly prepared in typescript form, are given in Table 1. Note that inclusive page numbers are to be given. Authors should ensure that the list of references includes all references mentioned in the paper and no others. The paper will not be sent to the printer until the list is complete.

All computer programs referred to in the paper should be included in the list of references. If the program is unpublished, the full address of the responsible author(s) should be given.

References occurring in the *Abstract* (§ 4) should be included in the reference list, even if the reference is not repeated in the body of the paper.

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. The Chemical Abstracts Coden reference for these *Notes for Authors*, for example, is ACACBN 39 174. Codens for many journals which are often referenced in structural papers are given in Table 2. Full details can be found in the *International Serials Catalogue* (1978), published by the International Council of Scientific Unions Abstracting Board. Codens-type references should not be included in the reference list at the end of the paper. The full list of references will be deposited. Other Codens, used by the data bases concerned, are acceptable alternatives, as long as their meaning is clear.

Table 1. *Examples of References*

The following references are laid out as an example of the correct format. They have, however, been reduced so as not to take up unnecessary space in these Notes.

Aikala, O. (1979a). J. Phys. C, 12, L581-L585.

Aikala, O. (1979b). Solid State Commun. 32,699-701.

Bednarz, B. (1977). Anharmonicity in Alkali Metals: An X-ray Approach with Particular Reference to Potassium and Lithium. PhD Thesis, Univ. of Adelaide.

Busing, W. R., Martin, K. O. & Levy, H. A. (1963). ORFLS. Report ORNL-TM-305. Oak Ridge National Laboratory,Tennessee.

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press.

Klepp, K. & Parthé, E. (1982). In preparation.

Koetzle, T. F. & Hamilton, W.C. (1975). Anomalous Scattering, edited by S. Ramaseshan & S. C. Abrahams, pp. 489-502. Copenhagen: Munksgaard.

Prince, E. (1982). Mathematical Techniques in Crystallography and Materials Science. New York: Springer.

Yamamoto, A. (1982). Acta Cryst. A38, 87-92.

8. Nomenclature

8.1 *Crystallographic nomenclature*

Atoms of the same chemical species within an asymmetric unit should be distinguished by an appended arabic numeral in parentheses. Examples are C(1), C(2), ...; N(1), N(2), ...; Ca(1), Ca(2), ...; Si(1), Si(2), ... Fully serial numbering, for example C(1), C(2), ..., C(18), N(19), N(20), ..., N(24), Ca(25), ... may be used when more convenient. Subscripts (C_1, C_2, C_3, *etc.*) are not acceptable, except as allowable under IUPAC/IUB rules, as they lead to confusion in chemical contexts. Hydrogen atoms, if not individually numbered, may be indicated in terms of the atom to which they are attached, *e.g.* H(C3), H'(C3), H''(C3), *etc.* If there is a standard chemical numbering of atoms, for example in a ring system, this numbering should be retained insofar as it can be made consistent with the other recommendations of this section.

Table 2. *Codens for journals frequently referenced in crystallographic papers*

ACACBN	Acta Cryst. A
ACAPCT	Acta Chem. Scand. A
ACBCAR	Acta Cryst. B.
ACIEAY	Angew. Chem. Internat. Edn
ACSCEE	Acta Cryst. C
AJCHAS	Austral. J. Chem.
AMMIAY	Amer. Miner.
ANCPAC	Ann. Chim. Paris
ANYAA9	Ann. N.Y. Acad. Sci.
BCSJA8	Bull. Chem. Soc. Japan
BSCBAG	Bull. Soc. Chem. Belges
BSCFAS	Bull. Soc. Chim. France
BULMD9	Bull. Miner.
CAMIA6	Canad. Miner.
CCACAA	Croat. Chim. Acta
CCCCAK	Coll. Czech. Chem. Comm.
CCNRAI	Cement and Concrete Res.
CHBEAM	Chem. Berichte
CHDCAQ	C.R. Acad. Sci. Paris Ser. C
CHINAG	Chem. Industry
CHPLBC	Chem. Phys. Letters
CIWYAO	Carnegie Inst. Washington Yearbook
CJCHAG	Canad. J. Chem.
CJPHAD	Canad. J. Phys.
CMLTAG	Chem. Letters
CPBTAL	Chem. Pharm. Bull. Japan
CRBNAH	Carbon
CSCMCS	Cryst. Struct. Comm.
CUSCAM	Curr. Sci. India
DANKAS	Dokl. Akad. Nauk SSSR
DANND6	Dop. Akad. Nauk Ukr. Ser. B Geol. Khim. Biol. N.
ECEMIM	European Cryst. Mtg
FCMLAS	Finnish Chem. Letters
GCITA9	Gazz. Chim. Ital.
HCACAV	Helv. Chim. Acta
ICHAA3	Inorg. Chim. Acta
INJADP	Indian J. Phys. A
INOCAJ	Inorg. Chem.
INUCAF	Inorg. Nucl. Chem. Letters
IVNMAW	Izv. Akad. Nauk SSSR Neorg. Mat.
JACGAR	J. Appl. Cryst.
JACSAT	J. Amer. Chem. Soc.
JBCHA3	J. Biol. Chem.
JCCCAT	J. Chem. Soc. Chem. Comm.
JCCMBQ	J. Coord. Chem.
JCDTBI	J. Chem. Soc. Dalton Trans.
JCMLB5	J. Cryst. Mol. Structure
JCOMAH	J. Less Common Metals
JCPKBH	J. Chem. Soc. Perkin Trans. II
JCPRB4	J. Chem. Soc. Perkin Trans. I
JFLCAR	J. Fluorine Chem.
JINCAO	J. Inorg. Nucl. Chem.
JMOSB4	J. Mol. Struct.
JMTSAS	J. Mater. Sci.
JOCEAH	J. Org. Chem.
JORCAI	J. Organomet. Chem.
JPCHAX	J. Phys. Chem.
JPFMAT	J. Phys. Sect. F
JPSCAU	J. Polymer Sci.
JPSLBO	J. Phys. Letters
JPSOAW	J. Phys. Sect. C Solid State
JRPSDC	J. Chem. Res. (Synopsis)
JRSPAF	J. Raman Spectr.
JSSCBI	J. Solid State Chem.
JSTCAM	J. Struct. Chem.
JUPSAU	J. Phys. Soc. Japan
KOKHDC	Koordinat. Khim.
KRISAJ	Kristallografiya
MNLMBB	Miner. Mag.
MOCMB7	Monats. Chem.
MPMTAG	Tschermak's Miner. Petr. Mitt.
MRBUAC	Mater. Res. Bull.
MSCEAA	Mater. Sci. Engineering
MSCJDS	Mater. Sci.
NATUAS	Nature
NATWAY	Naturwissenschaften
NJCHD4	Nouv. J. Chim.
NJMIAK	Neues Jahrb. Miner. Abt.
NJMMAW	Neues Jahrb. Miner. Monatsh.
PABAD5	Prog. Abs. Amer. Cryst. Ass. Mtg.
PCMIDU	Phys. Chem. Miner.
PHBCDQ	Physica A and B
PRBMDO	Phil. Mag. B
PSENAC	Photogr. Sci. Eng.
PSSABA	Phys. Stat. Solidi A
RADKAU	Radiokhimia
RTCPA3	Rev. Trav. Chim. Pays-Bas
RVCMA8	Rev. Chim. Miner.
SAMCAS	Spectrochim. Acta A
SCIEAJ	Science
SSCOA4	Solid State Comm.
TELEAY	Tetrahedron Letters
TETRAB	Tetrahedron
TMCHDN	Transition Metal Chem.
ZAACAB	Z. Anorg. Allgem. Chem.
ZEKGAX	Z. Krist.
ZEMTAE	Z. Metallkunde
ZENBAX	Z. Naturforsch. B
ZNOKAQ	Zh. Neorg. Khim.
ZOKHA4	Zh. Obshch. Khim.
ZPCFAX	Z. Phys. Chem. (Frankfurt)
ZSTKAI	Zh. Strukt. Khim.

When it is necessary to distinguish crystallographically equivalent atoms in different asymmetric units the distinction should be made by lower-case roman numerals superscript to the arabic numeral or to the chemical symbol if there is only one atom of a chemical species in the unit cell. Examples are C(1), C(1^{i}), C(1^{ii}), C(1^{iii}), C(1^{v}), C(1^{vi}), ..., Na(3^{ii}), Nd^{iv}, *etc.* Atomic designations should be consistent throughout the manuscript.

Space groups should be designated by the Hermann–Mauguin symbol, for example *Pba*2. Standard cell settings, as listed in *International Tables for X-ray Crystallography*, should be used unless objective reasons to the contrary are stated. Hermann–Mauguin symbols should also be used for designating point groups and molecular symmetry.

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 by the author. The symbol f' represents the real, f'' the imaginary dispersion term, in the scattering factor $f = f_0 + f' + if''$.

'Lattice' is a mathematical concept with an exact meaning, and should not be used loosely as a synonym for 'structure'. 'Centric' and 'acentric' refer to the intensity distribution arising from 'centrosymmetric' and 'non-centrosymmetric' structures, respectively, and not to the structures themselves. The proper names Fourier and Patterson should not be used as common nouns, nor should, for example, an electron-density projection be designated by the more general and therefore relatively ambiguous term 'Fourier projection'. For nomenclature recommendations on polytypism, syntaxy, topotaxy and epitaxy, see the Bailey recommendations in § 8.2.

8.2 *Nomenclature of chemical compounds etc. and minerals*

Names of chemical compounds and minerals are not always unambiguous. Authors should therefore quote the chemical formulae, including structural formulae for organic compounds, of the substances with which their papers deal.

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 (IUB) and other appropriate bodies. As far as possible the crystallographic nomenclature should correspond to the systematic name.

Any accepted trivial name, trade mark, recommended International Non-proprietary Name, United States Adopted Name or British Pharmacopoeia Approved Name may be retained, but the corresponding systematic (IUPAC) name should always be provided.

Authors should, if possible, give details of the origin, treatment, purity, and experimental density. It may be necessary to give the atomic weights of isotopes. For nomenclature of minerals and polytypes see Bailey *et al.* [*Acta Cryst.* (1977), **A33**, 681–684]. The Bailey recommendations may be superseded by the Guinier recommendations now under

consideration by the Nomenclature Commission and Executive Committee.

All papers in *Acta Crystallographica*, Section C, and all Crystal Data in *Journal of Applied Crystallography* should normally include (i) the approved name(s) of the compound(s) in the *Title* of the paper or in a footnote to the title and (ii) the chemical formula in the *Title*. Any paper in *Acta Crystallographica*, Section A or Section B, or in *Journal of Applied Crystallography* dealing with the crystal physics or the properties of a particular material should also include the approved name of the compound concerned.

For a list of available chemical nomenclature sources see *Acta Cryst.* (1979), **B35**, 2827 or *Chem. Int.* (1982), **5**, 15–19. [*Approved Names* 1977 – a list of approved names for pharmaceutical compounds with their corresponding systematic (IUPAC) names, published for the British Pharmacopoeia Commission – is available from Her Majesty's Stationery Office, London.]

Assistance in the naming of compounds in accordance with IUPAC and IUPAC–IUB rules may be obtained from Dr K. L. Loening, Director of Nomenclature, Chemical Abstracts Service, PO Box 3012, Columbus, Ohio 43210, USA; and in the particular naming of inorganic compounds from Professor Y. Jeannin, Laboratoire de Chimie des Métaux de Transition, Université Pierre et Marie Curie, 4 place Jussieu, 75230 Paris CEDEX 05, France. Enquiries may also be addressed to Dr J. E. Derry, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. If advice on chemical nomenclature is sought from the above advisory sources, authors are requested, when submitting a manuscript to the Union's journals, to indicate the source consulted.

8.3 *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 nanometer (nm) or picometer (pm). Recommended prefixes of decimal multiples should be used rather than '$\times 10^n$'.

Useful publications on the SI system are *A Guide to International Recommendations on Names and Symbols for Quantities and on the Units of Measurement* (1975) by D. Armstrong Lowe (Geneva: World Health Organization) and *Units of Measurement* (1979) (ISO Standards Handbook 2; Geneva: International Standards Organization).

8.4 *Abbreviations*

Abbreviations should be explained where they first appear in the text, unless they are commonly used and known by nearly all crystallographers or can be found in ordinary dictionaries of the language of the paper.

9. Typography

9.1 *Conventions for indicating type style*

The Technical Editor will normally indicate to the printer the style of type to be used, and it is better that authors should not indicate it at all rather than do so in a way different from that understood by the printers.

9.2 *Mathematics and letter symbols*

The printing of mathematics is much more expensive than printing ordinary text, and mathematical arguments should be abbreviated as far as is practicable without loss of clarity.

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. Vectors and tensors should be distinguished by a wavy underline.

Letters or signs that can be confused when handwritten (particularly a, d, α; I, I, l, l; u, n, h, η, μ; x, $\times$, X, χ, κ; v, r, ν, γ; σ, δ; 2, z; ξ, ζ; w, W, ω; E, ε, $\in$) should be very carefully distinguished by marginal notes if necessary. It is important to indicate whether capital or lower-case letters are intended when certain letters including the following are handwritten: C, K, O, Q, S, U, X, Z. Greek letters should not be spelled out except in marginal notes of clarification, and where a Greek capital letter is required, this should be stated unless it is clearly recognizable as such. Care should be taken not to cause confusion by using the same letter symbol in two different meanings. In connection with articles on diffractometry it is to be noted that there is no completely satisfactory way of distinguishing Greek capital chi from both lower case chi and Roman (or italic) capital X when all three are used together.

Gothic, script, or other unusual lettering should be identified in marginal notes. The Technical Editor may instruct the printer to use another type face if that indicated by the author is not readily available.

9.3 *Chemical and structural formulae*

Although some structural formulae can be set in type, authors should generally provide such formulae in camera-ready form (see § 5).

10. Computational details

Sufficient information should be given to permit the calculations to be repeated, or extended at any subsequent date by other workers, and to permit independent evaluation of the correctness and reliability of the analysis.

All measured or derived quantities which are of importance either to the conclusions or understanding of the paper, or to use by others, are required to be accompanied by their estimated standard deviations. The value of such quantities without estimated standard deviations is regarded as being sufficiently ill-defined as not to warrant publication.

The following recommendations apply specifically to the reporting of computations in structure determinations (see also Appendix I).

The wavelength or lattice parameter used as a standard for measurements of cell dimensions and also the temperature should be stated explicitly if the accuracy claimed or implied is better than 0·1%.

Structural papers will not be considered for publication unless accompanied by a legible table of numerical values of F_o and F_c (or an equivalent table of intensities if more appropriate). Values of h, k, l, F_o, F_c should be included in the table (see § 6.2); phase information is not necessary, but values of $\sigma(F_o)$ should be included unless calculable from a simple formula in the text. Reasons for omission of any reflexion with $\sin\theta < \sin\theta_{max}$ should be given.

All parameters involved in the final calculation of structure factors should be stated. The atomic scattering factors used should be specified precisely (including corrections for anomalous scattering if applied). The weighting scheme adopted in least-squares calculations should be specified

(including a statement concerning any reflections given zero weight). A final agreement index or residual, R, based on all measured reflections, should be defined and quoted. The treatment of multiplicities, of reflections measured as zero or negative, and of reflections with $\sin\theta < \sin\theta_{max}$ but not measured, should be carefully specified.

When practicable, the correctness of the structure analysis should be supported by the agreement of two or more different methods of assessing the differences between model and actual structure, *e.g.* least-squares results and electron-density difference syntheses. The degree of completeness of the refinement calculations should be indicated, by giving, for example, the average and maximum parameter shifts as fractions of the e.s.d.'s in the final cycle of computations. Where corrections for torsional oscillations, *etc.* are made, the molecular dimensions before and after correction should be given.

Estimated standard deviations with a zero value for varied atomic parameters are not accepted and in such cases at least one additional place of decimals must be presented in the value of the quantity concerned together with the corresponding nonzero estimated standard deviation. If the parameter is invariant, it should be so designated and presented without estimated standard deviation.

Chemical-connectivity relationships in crystal structure manuscripts are often calculated from coordinates containing more decimal places than are given in the table of atomic parameters. All such relationships, including bond lengths, bond angles and torsion angles, must be calculated without significant truncation from the unit-cell dimensions and atomic coordinates given in the manuscript.

Anisotropic thermal parameters are to be published only if the table of values is very short, or they are necessary for understanding the paper, or they possess unusual features. In all other cases, the table of values is to be deposited: a brief discussion of deposited values should instead be presented, including the maximum and minimum values found and the presence of any nonpositive-definite coefficients determined. In addition, the equivalent values of the Debye–Waller factor should be given for publishing with the list of atomic coordinates. Estimated standard deviations on such equivalent values are not required. The presence of unusual anisotropy should be referred to in the text (including any nonpositive-definite coefficients found), or in the table of B_{eq} (by use of an asterisk), or illustrated by a plot of the atomic vibrational ellipsoids (see § 5.1).

When absorption, extinction, or any special corrections or scale factors are applied in the reduction of the intensity data, the method used should be described and maximum and minimum corrections stated together with such details of crystal shape and orientation to allow the reconstruction of the actual ray paths.

Routine checking of papers containing structural data, for consistency between the atomic coordinates and lattice constants and the quoted bond lengths, bond angles and torsion angles, is carried out by all Co-editors. Since the detection of inconsistency will result in a paper being returned to its authors, care should be taken to ensure that the final tables and results presented in the manuscript correspond accurately to the primary data. Crystal structure papers must be accompanied by the connected computer output of the author's program that lists all final input data together with the output bond lengths and angles, if required by the Co-editor to whom the paper is submitted. All numerical information on the computer output must be clearly labelled. In addition, the first sheet of the structure factor listing should be given as part of the continuous listing if possible.

All computer programs used in the crystallographic analysis should be identified both in the text and in the reference list, as specified in § 7.

11. Supplementary publication procedure (deposition)

11.1 *Purpose and scope*

Some parts of some papers are of interest to only a very small number of readers, and the high and increasing cost of printing these parts is not warranted. The International Union of Crystallography has therefore arranged for the preservation of such material at the British Library Lending Division (as full-sized copy or microfiche) and for material on macromolecular compounds with the Brookhaven Protein Data Bank (in machine-readable form).

For papers in *Acta Crystallographica*, Sections A and B and for papers other than Crystal Data in *Journal of Applied Crystallography*, the information to be deposited is at the discretion of the Co-editor and may include the following.

(i) Details of the experimental procedure.

(ii) Details of the stages of structure refinement, see also the requirements for papers in *Acta Crystallographica*, Section C, below.

(iii) Details of mathematical derivations given only in outline in the main text, and in mathematical Appendices.

(iv) Lengthy discussion of points that are not of general interest or that do not lead to definite conclusions but that do have significant value.

Authors should indicate clearly those parts of their paper intended for deposit. Acceptance of a paper may be conditional on the deposit of further parts. All material to be deposited is subject to the usual refereeing procedure.

For papers in *Acta Crystallographica*, Section C, the following data will be deposited:

(i) Structure factors and anisotropic thermal parameters, including estimated standard deviations, except as provided in § 6.1. Weak reflections classified as unobserved should be included. (Atomic coordinates, thermal parameters, if determined, and structure factors will also be deposited for macromolecular papers, see § 11.2.)

(ii) Least-squares planes and deviations from them with few exceptions.

(iii) Calculated hydrogen-atom coordinates unless they are necessary to the understanding of the paper.

(iv) Normal intermolecular distances.

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

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 (see Appendix III).

For Crystal Data in *Journal of Applied Crystallography*, the whole paper, with the exception of the *Title, Abstract* and acknowledgements, will be deposited. In addition, where appropriate the data will be checked by the Joint Committee on Powder Diffraction Standards (JCPDS) before publication and assigned a JCPDS reference number, which will be published as part of the *Abstract*. This will mean that the powder pattern will be published in the Powder Diffraction File at the earliest date possible.

As most biological-macromolecule structural investigations currently pass through several stages of improving resolution and the required deposition and resulting public availability of the structure factors may deprive the investigator of a hard-earned advantage, an author who expects to be disadvantaged by having his list of structure factors made generally available may request that this list be granted a privileged status for a period no longer than four years from the date of publication. Earlier release of such would require the specific consent of the authors.

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.

11.2 *Deposition procedure*

If deposition is in hard-copy form, then the material should be prepared as described in the following section and sent in triplicate with the paper to the Co-editor, who will send copies on for deposition when he transmits the paper to the Technical Editor.

If authors wish to deposit their data in the form of microfiches, they should still submit full-size copy in triplicate to the Co-editor for refereeing purposes. At the Co-editor's request, the Technical Editor will supply a Supplementary Publication Number (SUP ...), which, with the authors' names and the *Title* of the paper or the compound name, should form the eye-readable *Title* of the fiches.

If the structure determination is of a macromolecule, any substance containing a polypeptide, polynucleotide or polysaccharide chain longer than 25 residues, deposition is to be in machine-readable form with the Brookhaven Protein Data Bank. The manuscript should be accompanied by printed copies of the atomic coordinates which will be sent to the referees. Then the Co-editor will request the authors to send the appropriate data to the Data Bank. The Protein Data Bank will acknowledge receipt of the machine-readable data both to the author and the Co-editor and will, at the same time, communicate to both the reference number assigned to these data. As soon as the data have been processed into standard Data Bank format and the corresponding listings verified by the author, notification will be sent to the Co-editor. Such listings can usually be prepared in less than one month, with the cooperation of the author. Final acceptance of the manuscript requires that the atomic coordinates and structure factors have indeed been satisfactorily processed by the Data Bank, although the paper will be typeset if otherwise acceptable. The data will also be deposited, as microfiche produced by the Protein Data Bank, with the British Library under the IUCr Supplementary Publication Scheme.

Magnetic tape with fixed line length and fixed block size in 7 track, BCD, 200, 556 or 800 CPI; or 9 track, ASCII or EBCDIC, 800, 1600 or 6250 CPI; or punched cards with IBM 026 or IBM 029 codes; or paper tape, 8-level ASCII code are equally acceptable machine-readable media for deposition. Each deposition should be accompanied by sufficient information to allow ready transcription of the medium, such as a FORMAT statement and a designation of the recording equipment used.

11.3 *Preparation of hard copy for deposit*

Material for deposit (in hard-copy form) should be of a quality such that photocopies of it are completely legible. Blue typewriter ribbons and blue print should be avoided. Generally, the dimensions of all text and tables intended for deposit should not exceed the dimensions of the A4 International Paper Size (210 × 297 mm), although the paper size may be greater. Larger dimensions (up to 390 × 285 mm) may be acceptable under exceptional circumstances. In such cases, the author should reach prior agreement with the Technical Editor.

The material for deposit must not be photographically reduced beyond the point at which the individual characters would be substantially smaller than those of normal typescript (minimum character height 1·5 mm). The information density in deposited material should, however, be reasonably high. A single column of values, for example, particularly if it continues for many pages, may be returned to the author for reformatting.

The first page of a deposit should consist of the title page of the paper to which it relates, including the *Title* and *Abstract* of the paper and the authors' names and addresses. Tabular matter should be headed descriptively on the first page, with column headings recurring on each page. Pages should be clearly numbered to ensure the correct sequence.

11.4 *Procedure for obtaining copies of deposits*

Copies of material deposited with the British Library may be obtained, free of charge, from the Executive Secretary of the International Union of Crystallography, whose address is given, as News and Meetings Editor, on the inside front cover of all issues of *Acta Crystallographica* and *Journal of Applied Crystallography* and in the footnote giving the Supplementary Publication Number of each deposit. This Number must be quoted in any request for copies of deposited material.

Copies of data in machine-readable form for macromolecules are available, unless the author has requested privileged status, see § 11.1, from the Protein Data Bank at Brookhaven or one of the affiliated centres at Cambridge, Melbourne or Osaka.

APPENDIX I

Criteria for publication in *Acta Crystallographica*, Sections B and C, and format for papers to be published in Section C

Papers will only be considered for publication in Section B of *Acta Crystallographica* if they meet the following three criteria:

1. The paper must contain a major structural element. This component may be an original determination of one or more structures (a single structure should generally have been studied under more than one condition of temperature or pressure), a theoretical structural investigation including new methodology, or a study of structural relationships based on a search of the literature. The calibre of this component should be at least as high as was previously required for acceptance in Section B up to 1982.

2. The paper should also present an experimental and/or theoretical contribution to one of the natural sciences that is novel, original and of high quality.

3. The paper should combine these two types of contribution to provide new structural insight for that science or for crystallography.

Papers which present the results of a crystal structure determination or of several such determinations, but are concerned with the crystal and molecular structure alone, will only satisfy the first of these criteria and will therefore be considered for publication in Section C.

Subject to the Co-editor's discretion, papers submitted for consideration in *Acta Cryst.*, Section C should conform with the following arrangement [*Acta Cryst.* (1981), **B38**, 699–700]:

The *Title* will consist of the name of the substance and the chemical formula; a qualification such as 'Structure of . . .', 'New Form of . . .', 'from Minas Gerais' *etc.* may be added.

The *Abstract* will consist of the information given in Table 3(*a*) (in abbreviated telegraphic form and preferably in the order given there).

The *Introduction* will briefly state the reason for undertaking the structure determination and its chemical, physical, biological or other interest. If organic, or containing complicated organic ligands, a display of the structural formula of the material studied should be given, in accordance with IUPAC convention.

The *Experimental* section will include the information given in Table 3(*b*), given in tabular or abbreviated telegraphic form. Any further details, say of refinement, should be treated as normal text, but kept as brief as possible.

The *Discussion* will generally include two tables and two figures as described in § 2.1, although bond distances and angles may be shown on a figure if this is reasonably compact (see also § 5.1). Additional tables and figures may be deposited. If the table of bond distances and angles is very long, this will be deposited and only values that are unusual and relevant to the discussion will be given for publication. Comment should be made on any unusual features of coordination, bonding, bond lengths, bond angles, thermal vibrations, *etc.*

Any nonroutine measurement of physical properties (magnetic susceptibility, dielectric permittivity, elastic moduli, *etc.*) should be mentioned in the *Abstract* and the numerical values quoted there if possible. If the numerical values are too lengthy to be given in the *Abstract*, they should be given in a suitably headed paragraph in the paper, normally preceding the *Discussion*.

Tables of structure factors, anisotropic thermal parameters, least-squares planes and hydrogen-atom coordinates if not refined must be submitted in triplicate with the paper, but will not normally be published. After acceptance of the paper they will be deposited along with any other extensive tables or figures, in accordance with the Union's procedures (see § 11).

Table 3. *Information required in* (*a*) *the Abstract and* (*b*) *the Experimental section of papers in Acta Crystallographica Section C*

(*a*) *Abstract*
- Formula weight
- Space group
- Unit cell dimensions
- Volume of unit cell (Å^3)
- Z
- Measured and calculated densities D_m, D_x
- Radiation and wavelength
- Linear absorption coefficient
- $F(000)$
- Temperature of measurement
- Final value of $R = [\sum (||F_o| - |F_c||)/\sum |F_o|]$ and number of unique reflections
- Source of material
- + such other material (especially structural) as can be conveyed in about 50 further words.

(*b*) *Experimental section*
- Method of measuring D_m
- Crystal shape and size
- Diffractometer used
- Number and θ range of reflections used for measuring lattice parameters
- Absorption correction applied (with maximum and minimum values)
- Maximum value of $(\sin\theta)/\lambda$ reached in intensity measurements
- Range of h, k and l
- Standard reflections and their intensity variation throughout experiment
- Number of reflections measured
- Number of unique reflections
- Value of R_{int} [$\sum (I - \langle I \rangle)/\sum I$, from merging equivalent reflections]
- Number of unobserved reflections
- Criterion for recognizing unobserved reflections [$I < n\sigma(I)$]
- Method used to solve structure
- Use of F or F^2 magnitudes in least-squares refinement
- Methods of locating and refining H atoms if applicable
- Parameters refined
- Values of $R = \sum (||F_o| - |F_c||)/\sum |F_o|$, $wR = [\sum w(|F_o| - |F_c|)^2/\sum wF_o^2]^{1/2}$ and $S = [\sum w(|F_o| - |F_c|)^2/(m - n)]^{1/2}$ (or the F^2 equivalents)
- Method used to calculate w
- Ratio of maximum least-squares shift to error in final refinement cycle
- Maximum and minimum height in final difference Fourier synthesis
- Secondary extinction value (if used)
- Source of atomic scattering factors and f', f'' values
- All computer programs used

APPENDIX II

Format for 'Crystal Data'

Contributions for the section Crystal Data of *Journal of Applied Crystallography* will be deposited under the Supplementary Publication Scheme and only the *Title*, names and addresses of the authors, *Abstract* and acknowledgements will be published. They must be in the following form (headings under which nothing would appear should be omitted):

(New) crystal data for . . .

[The *Title* may be preceded by an adjective (New, Revised, . . .) if appropriate.] The name and the chemical formula of the compound should be given in the correct IUPAC form.

Abstract

Do not repeat information in the title. Give (if applicable) the mineral name and locality, the chemical purity, space group (if known), the unit-cell parameters, the volume of the unit cell, Z, the measured and X-ray densities, measurement technique and conditions, radiation used and a description of the powder data and other data deposited. The unit-cell parameters, the volume of the unit cell and the measured density should each be accompanied by their e.s.d.

If powder data are included the JCPDS file number will be added before publication.

Origin of specimens

State method of preparation or, if naturally occurring, source and relevant details of extraction, or locality of origin for minerals.

Chemical characterization

Include, in tabular form, results of chemical analyses and their source.

Crystal geometry

State observed diffraction criteria: Laue class and space group (Hermann–Mauguin symbol) if determined.

State diffraction method with radiation and numerical value used for the wavelength.

Powder data

Give as much of the information as possible described in Appendix III.

Crystal morphology

List such data as goniometric axial ratio(s) and angles; crystal forms and form combinations; habit, malformation; cleavage(s) (Miller indices, quality, and facility) or fracture; twinning (twin law and composition surface); gliding; parting.

Crystal physics

List the data determined for physical properties such as:

Optical properties: indices, measured 2V, dispersion, optical orientation (use $\alpha\beta\gamma$ in preference to XYZ notation), pleochroism, *etc.*

Second-harmonic-generation characteristics

Melting point

Pyro- and piezoelectric properties; electrical, dielectric and elastic properties, magnetic susceptibility, spectra (infrared, NMR, *etc.*)

Diaphaneity, colour, streak, lustre, hardness, *etc.*

Other physical properties.

Comparison with other results

State succinctly whatever can usefully be said.

APPENDIX III

Standards for the publication of powder profile fitting (Rietveld) analyses and of powder pattern data

Suggested guidelines for the presentation of results of powder profile fitting analyses have been published in *Journal of Applied Crystallography* [Young, R. A., Prince, E. & Sparks, R. A. (1982). *J. Appl. Cryst.* **15**, 357–359].

Table 4. *Example of completed data form: powder diffraction data for phase characterization*

Data from Swanson, H. E. *et al.* (1971). *NBS Monograph* No. 25, Section 9, p. 25.

Bold-face items are considered essential.

Sample characterization

Name (chemical, mineral, trivial) **Magnesium aluminum oxide (spinel)**

Empirical formula $MgAl_2O_4$

Chemical analysis No × **Yes**

Source/preparation Synthetic; fusion of binary oxides

Chemical Abstracts Registry No. 12068-51-8

Pearson phase designation cF56

Other **Index of Refraction = 1·718 (Isotropic)**

Technique

Radiation type, source X-rays, Cu **λ value used** 1·54056 Å $K\alpha_1$

λ Discrim. (Filters, mono, *etc.*) Diffracted beam, curved LiF mono

λ Detector (Film, Scint., Position-sensitive, *etc.*) Geiger

Instrument description (Type, Slits, *etc.*) 17 cm vertical diffractometer

Div 1° Rec 0·003″

Soller Yes **No.** 1 **Position** Inc. **Aperture** q = 1·2

Instrumental profile breadth 0·10 °2θ **Temp. (°C)** 25 ± 1

Specimen form/particle size

Edge loaded powder/< 10 μm particle size for *I*'s, packed for 2θ's

Range of 2θ from 5 °2θ **to** 165·0 °2θ **Specimen motion** None

Internal/external 2θ std (if any) Ag (internal)

Lattice parameter of 2θ std 4·08641 Å

2θ error correction procedure Linear interpolation from nearest 2θ's of std.

Intensity meas. technique Strip chart record (peak heights)

Error (~) 5% **Peak** × **Integrated**

Minimum intensity threshold (in relative intensity units) 0·3

Intensity std used α-Al_2O_3 *hkl*'s of intensity std 113

Intensity ratio I/I_c 1·70 (5) Conversion factor if corundum not used

Resolution (FWHM) for this material: 0·10 °2θ at 59·37 °2θ

2θ reproducibility for this material: ±0·02 °2θ at All °2θ

Unit-cell data

Method of cell detn. Cell and structure known from Bragg (1915)

Cell refinement method Least-squares. See Appleman & Evans (1973)

a = 8·0831 (1) Å; b = ( ) Å; c = ( ) Å

α = ( )°; β = ( )°; γ = ( )°.

Z = 8; D_m = ( ) Mg m^{-3}; D_x = 3·578 Mg m^{-3}; V = 528·12 (2) Å^3;

Formula Wt. = 142·25

Crystal sys. Cubic Space group $Fd3m$ [227]

Crystal data index No. 8·0831

Figure of merit type F_N. See Smith & Snyder (1979)

Value F_{29} = 58 (0·015, 33)

References

APPLEMAN, D. E. & EVANS, H. T. (1973). NTIS Document No. PB-216188.
BRAGG, W. H. (1915). *Nature* (*London*), **95**, 561.
SMITH, G. S. & SNYDER, R. L. (1979). *J. Appl. Cryst.* **12**, 60.

( ) indicates standard deviation in least significant digit(s).

Table 5. *Presentation of powder data*

Information in the first two columns is essential, that in the remaining three columns is desired (see text).

2θ exp (°)	I/I_0	d_{exp} (Å)	*hkl*	$\Delta 2\theta$* (°)
19·02	35	4·66	111	+0·019
31·27	40	2·858	220	−0·003
36·84	100	2·437	311	−0·009
38·53	3	2·335	222	−0·021
44·83	65	2·020	400	+0·016
55·64	9	1·650	422	−0·020
59·37	45	1·5554	511	+0·008
65·24	55	1·4289	440	−0·001
68·64	3	1·3662	531	+0·006
74·13	3	1·2780	620	+0·003
77·32	8	1·2330	533	−0·029
78·40	1	1·2187	622	−0·013
82·64	5	1·1666	444	+0·006
85·76	2	1·1320	711	−0·012
90·97	5	1·0802	642	−0·009
94·10	12	1·0524	731	−0·005
99·34	7	1·0104	800	−0·006
107·90	2	0·9527	822	−0·020
111·22	8	0·93343	751	−0·014
112·32	1	0·92738	662	−0·035
116·91	6	0·90384	840	−0·025
120·50	1	0·88722	911	+0·004
121·69	0·9	0·88203	842	−0·021
126·76	0·8	0·86161	664	+0·013
130·74	8	0·84737	931	−0·011
138·07	17	0·82488	844	+0·033
142·97	0·4	0·81232	933	+0·024
152·70	2	0·79266	10,2,0	−0·033
160·65	11	0·78139	951	+0·025

* $2\theta_{exp} - 2\theta_{calc}$.

Other papers that present powder pattern data submitted for publication in IUCr journals are now required to follow the standards published in *National Bureau of Standards Special Publication* 567 (1979); a summary has been published [*Acta Cryst.* (1981). A**37**, 443–444; *J. Appl. Cryst.* (1981). **14**, 216–217].

The information requested by the standard data-form, a completed example of which is given in Table 4, must be given as compactly as possible. Essential information is requested by the bold-face headings. The remaining information sought is highly desirable, although it is recognized that some may not be available in all cases. Partial omission of the optional data will not preclude publication of the paper. Powder data corresponding to the information given in Table 4 are presented, in the preferred form, in Table 5. Reprints of the complete standard, including copies of the blank data-form, are available from any Co-editor.

Among the requirements for reporting powder diffraction data are:

(*a*) The published powder pattern should be as complete as possible and should include weak as well as strong diffraction lines. Where possible, the data should extend to at least 100 °2θ (Cu $K\alpha$ radiation). Patterns with a small number of lines should extend to the limit of the experimental method used.

(*b*) The experimentally observed 2θ values should be given in degrees, corrected for systematic instrumental error.

(*c*) Intensities should be reported numerically, with the most intense line scaled to 100 and intensities less than 1 reported as decimal fractions. Intensity values reported should not imply a precision greater than that measured.

(*d*) The reproducibility of the measured values of 2θ and I should be indicated, as obtained by multiple mountings of the sample material.

(*e*) Indexing of the powder diffraction data is required for all but the rarest and best-defended cases. Authors should report a figure of merit based on the accuracy of the 2θ measurements and the completeness of their data.

(*f*) Information concerning line breadth of the sample should be supplied.

(*g*) Additional information of value to future users should be supplied, such as the standard deviations, Chemical Abstracts Service Registry number, Crystal Data index number, *etc.*

To justify being published, powder diffraction data must constitute an original contribution to the literature. As an original contribution, the data must be the first published for a well-characterized phase, must be a significant correction to or an improvement on published data, or must relate to the phase in a previously uncharacterized condition, *e.g.* at elevated temperature or pressure. A powder pattern calculated from single-crystal structure data does not in itself meet the criterion of originality.