International Union of Crystallography

Notes for Authors

Contents

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 two sections. Section A is devoted to crystal physics, diffraction, and theoretical and general crystallography, Section B to structural crystallography and crystal chemistry. The *Journal of Applied Crystallography* is concerned with application of crystallography and crystallographic techniques, other than crystal-structure determination, and to the apparatus, techniques and other factors involved.

Both journals publish contributed articles, Short Communications, and Book Reviews. Occasional review articles are welcomed. In addition, the *Journal of Applied Crystallography* publishes Reference Information and Comment. Details of these various categories and remarks on interim reports are given in Appendix I.

The editors of the journals cooperate closely. If a paper submitted to one of the journals is considered to be more appropriate to the other, the author(s) will be consulted, and the transfer accomplished without loss of the original date of receipt.

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 a list giving the names and addresses of the editors (Editor and Co-editors)

and the Technical Editor. Manuscripts are to be submitted to one of the editors, but not to the Technical Editor, who deals with manuscripts only after they have been accepted by one of the editors.

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. In cases of difficulty, contributions in any of the four languages may be submitted to the Editor.

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 this 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 of the authors.

1.4 *Copyright*

Every manuscript should be accompanied by a statement transferring copyright, except as required otherwise by national laws, from the authors (or their employers – whoever holds the copyright) to the Union; the form for copyright transfer is printed at the end of these *Notes for Authors* and copies are also available from any of the editors or from the Executive Secretary of the Union. This written transfer of copyright (including material deposited in accordance with § 10), which previously was assumed to be implicit in the act of submitting a manuscript, has become necessary, because of recent changes in copyright laws, in order for the Union to continue to disseminate the results of crystallographic research as widely as possible. A more detailed explanation of these changes and the need for written transfer of copyright is given in the first issues of *Acta Crystallographica* (p. 158 at the end of these *Notes*) and *Journal of Applied Crystallography* for 1978 under the heading *International Union of Crystallography, Transfer of Copyright*. Further information may be obtained from the Executive Secretary of the Union.

1.5 *Preparation and handling*

The editor to whom a paper is submitted is reponsible for choosing referees and for accepting or rejecting the paper. If the paper is accepted it is the responsibility of the Technical Editor to prepare the paper for printing; in this connection he may have to correspond with authors in order to resolve ambiguities or to obtain satisfactory figures or tables. The handling given to a manuscript is described in § 11.1 below.

Authors are requested to give particular attention to the details of preparation outlined in the following paragraphs. Authors of crystal-structure papers may find useful the check list in Appendix VI.

2. Typescripts

2.1 *Paper, margins, spacing, general style*

Contributions should be typed on one side only of good quality paper of normal size, should (except as indicated in § 5) be double-spaced (*not* $1\frac{1}{2}$-spaced) or triple-spaced (at least 8 mm, centre to centre, between lines) with wide margins, and should conform to the general editorial style of the journal. The purpose of the wide spacing and margins is to leave adequate room for all needed editorial changes and for the Technical Editor's instructions to the printer. It is particularly important that much space for editorial instructions be left in the list of references (§ 6 and Appendix II), tables to be set in type (§ 5), figure captions, and the heading of the paper. Clarity for the printer is essential; elegance, in itself, is not.

2.2 *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.

2.3 *Use of marginal notes for clarification*

Unconventional usages or possible ambiguities (for example, zero and the letter O, especially when subscript; indices *hkl* or *hkl*; Greek letters and special symbols) should be explained in marginal notes (see also § 8.2).

2.4 *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.

Every typescript should bear, on the first page, the name and full postal address of the person to whom the proofs and reprint order form should be sent. In the absence of other written instructions *on or with the typescript* these will be sent to the first-named author at the address given in the heading of the paper.

2.5 *Number of copies*

Manuscripts (including all figures and tables) should preferably 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.

2.6 *Manuscript length*

Brevity of presentation is essential. Only exceptionally can papers be considered which exceed about 6000 words. Articles intended for publication as Short Communications should not exceed the equivalent of about 1000 words. The primary consideration, however, is one of density of information: often the information contained in several related short papers can be presented more concisely in a single longer paper.

Information in the title (name of substance, formula, mineral locality, . . .) should be omitted from the abstract for the sake of brevity, and information in the abstract (cell dimensions, density, . . .) should not be unnecessarily repeated in the body of the paper. Effective use should be made of tables and figures to reduce the overall length of the manuscript; redundancy between figures, tables and text should be avoided (§§ 4.1, 5.1).

2.7 *Supplementary material*

When an author refers to other works of his not currently available from major libraries throughout the world, two copies of those works should be submitted for the use of the referees. Similarly, submission of additional tabular material, computer output, listings, *etc.*, that could be of help to the referees is encouraged. Materials intended for deposit should be prepared in accord with § 10.

3. Title and abstract

3.1 *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, for example by the full chemical name, by the trivial chemical name and an adequate formula, or, in the case of a mineral, by the mineral name and locality.

3.2 *Abstract*

Each contribution subject to refereeing (ordinary articles, Short Structural Papers, Short Communications, Crystal Data, Computer Programs; see Appendix I) 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 and should be written in the third person. It should not repeat information given in the title. Ordinarily 200 words suffice for a full paper and 100 words for shorter contributions. It should make no reference to tables, diagrams or formulae contained in the paper.

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.* [Helmholdt & Vos (1974). *Acta Cryst.* A**33**, 38–45].

A format is prescribed for the abstracts of Short Structural Papers (Appendix IV); this will serve as a guide for the abstracts of most structural papers in other categories.

For the abstracts of Laboratory Notes see Appendix I; for those of Crystal Data see Appendix V.

An author whose national language can be printed in Roman or Cyrillic characters but is not one of the four languages of publication (§ 1.2) may, in addition, give a brief summary in his national language at the end of the paper.

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 Co-editors on request.

4. Diagrams and photographs ('figures')

4.1 *Need*

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, it is preferred that bond lengths and bond angles should be indicated in a simple 'ball-and-stick' figure whenever this is consistent with clarity; the corresponding table should then be omitted entirely or, if the author prefers, deposited *via* the auxiliary publication procedure (§ 10). Unless they contribute to the conclusions, such as in studies of thermal motions and structural disorder, thermal-ellipsoid diagrams should be deposited or omitted. Neither a ball-and-stick nor a thermal-ellipsoid figure is a satisfactory substitute for an organic structural formula, unless double bonds, hydrogen atoms *etc.* can be included without loss of clarity.

Supplementary diagrams are acceptable for deposit under the auxiliary publication procedure (§ 10).

4.2 *Quality, backing, colour*

Diagrams must be provided in 'hard copy' form, that is, as carefully made original 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 (such as some types of tracing paper and tracing plastic) or in size so large that they are rolled or folded.

If they meet the other requirements, good quality reduced photographic copies of large diagrams are perfectly satisfactory and are easier to handle 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. In many cases it will be helpful if the author will indicate which features of the photograph should be reproduced most faithfully. Plates in colour are accepted only if the entire cost is paid for by the author or his organization. In exceptional circumstances authors may be asked to contribute to the cost of monochrome plates on art paper.

4.3 *Size*

Diagrams should be as small as possible consistent with clarity. They will usually be further reduced by the printer, preferably so that the greatest width 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). Diagrams requiring more than one column width will not be accepted for Laboratory Notes.

In planning their diagrams to accord with the column width of the journal, authors are reminded to make allowance for space taken up at the sides by lettering.

Note: The maximum area available for printing on one page is 165 mm × 220 mm. Examples of convenient widths for original drawings (including lettering) intended for reduction to page or column width are 220 mm (reduction to $\frac{3}{4}$) and 160 mm (reduction to $\frac{1}{2}$) respectively. In calculating the maximum allowable height for an original diagram, make allowance for the estimated height occupied by the legend which is to be printed underneath. Allow 5 mm on the printed journal page for the first line of the legend and a further 3 mm for every additional line.

Originals requiring excessive reduction should not be submitted.

Related diagrams (for example, several projections of the same structure) should ordinarily be presented on the same scale.

Diagrams intended for stereoscopic viewing must be submitted on the correct scale with approximately 55 mm between centres, ready to be published without size reduction or change of separation. Atom labelling should be included on both left and right views in stereo perspective.

4.4 *Lettering and symbols – size and placement*

Fine-scale details and lettering must be large enough to be clearly legible (not less than 1 mm in height) after the whole diagram has been reduced to an economical printed size, often to one column (80 mm) or less width. Lettering should be kept to a minimum: descriptive matter should be placed in the legend rather than in the diagram.

4.5 *Lettering and symbols – camera-ready copy*

On diagrams and figures, the authors' own lettering ready for photographing is preferred if it is neat, is of suitable size to be clearly legible in the possibly much-reduced size in which the figure will finally be printed, is reasonably consistent with the style of the journals, is securely fixed in place, and meets the following criteria: Single letters denoting vectors should be in heavy type without arrows, other letter symbols (except those for names of units) in italics or 'Porson' (sloping Greek), and other lettering normally in ordinary type. Symbols denoting units should be in the usual style of the journal and, when given on ordinate or abscissa scales, they should be included in round brackets. Letters (*a*), (*b*), *etc.* identifying separate diagrams in a group collected together over a single legend should normally be placed below (never above) the diagrams to which they refer.

4.6 *Lettering and symbols – optional indication*

Lettering may be indicated in soft pencil or on a second copy of the diagram, but all other features, including such details as arrows, arcs, or broken lines, must be ready for photographing; the editors cannot arrange for missing or poorly presented details to be added or redrawn. Pencilled lettering must be placed on the diagram in such a way that the printers can readily affix printed characters of generous size without obscuring parts of the diagram itself. Neatness and legibility of pencilled lettering are essential; mistakes lead to additional expense and delay. Special care is necessary to avoid confusion between certain letters (see § 8.2, below, on *Mathematics and letter symbols*).

4.7 *Numbering and legends*

Diagrams and photographs are to be numbered as figures in a single series, normally in the order in which they are referred to in the text. Every figure must have a legend to be printed below it with the figure number. A list of the legends ('figure captions') in double spaced typescript is to be attached to the manuscript. In both the list and in the text, the abbreviation 'Fig.' is used when figures are identified by number.

5. Tables

5.1 *Economy in use of tables*

Although extensive numerical information is most economically presented in tables, diagrammatic representation of bond lengths and bond angles is preferred when possible. Authors should ensure that the text and diagrams are not redundant with the tables.

5.2 *Treatment of tables*

Tables forming part of papers accepted for publication may be handled in three ways:

(i) they may be set in type by the same process as the rest of the paper.
(ii) They may be reproduced photographically.
(iii) They may be deposited in accordance with the auxiliary publication procedure (§ 10).

For reasons of economy, small tables will normally be set in type while large tables either will be photographically reproduced or will be deposited. Structure-factor tables and tables of anisotropic thermal parameters are deposited, except when very short or when the nature of the paper requires that they be immediately available.

5.3 *Design, size, accuracy*

Every table 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; excessive space between columns, for example, is discouraged. Tables of, for example, positional parameters should be prepared in such a way that they do not require the printing of large numbers of zeros. Tables to be photographed should be typed in single spacing. Tables which appear to be wasteful of space will be returned to the authors for reconstruction, with consequent delay in publication.

Tables should be prepared on sheets no larger than those used for the typescript. Large tables that will be photographically reproduced for publication should be photographically reduced to convenient size before submission. Tables for deposit, on the other hand, should not be photographically reduced very much (see § 10.3) and hence must be arranged in multiple-page style. Authors should check that the prints submitted are clearly legible in every part and are free from errors, ready for photographic reproduction.

5.4 *Structure-factor tables*

Structure-factor tables to be deposited must conform to the requirements of the auxiliary publication procedure (§ 10.3).

Structure-factor tables to be published with the paper are reproduced photographically unless very short (§ 5.2). The density of structure factors in tables for publication should be not less than 2000 per journal page. They must therefore be presented in clear black type and must be in single spacing (not double spacing as required for manuscripts). They should be designed so as to conform, after the reduction indicated below, to the dimensions of a page or column of the journal. The reduction given to F tables will be such that the figure 1 is not more than about 0·8 mm in height. The width available for printing is to be taken as 165 mm or (for a single column of the journal) 80 mm. Tables of F values which are unsuitable for reduction to 80 mm width but are considerably less than 160 mm wide after a reasonable reduction, or are for any other reason considered by the editors to be wasteful of space, may be returned to the author for rearrangement. The editors reserve the right to reduce tables to the extent that a lens is necessary for reading.

Tables of F values should be of the same width from top to bottom, with columns properly aligned and as close together

as is reasonably practicable. Tables which satisfy the foregoing requirements may be of any height after reduction, provided only that no single page or column may then exceed 220 mm in height, including headings *etc.* which are to be set in type by the printer. The minimum allowance needed for these is 5 mm of height for every printed line of the main caption plus 4 mm for each line of headnotes; for footnotes to be set in type, an allowance similar to that for headnotes must be made.

Column headings in F tables must be ready for photographing, but as an alternative they may be omitted and the columns explained in a headnote. It is recommended that values of h, k, l, F_o, F_c be included in the table; phase information does not seem necessary, but the editors welcome the inclusion of $\sigma(F_o)$ or $\sigma(|F_o|^2)$ unless it is calculable from a simple formula in the text. Reasons for omission of any reflexion with $\sin\theta < \sin\theta_{max}$ should be given.

6. References

References to published work must be indicated by giving the appropriate authors' names (in parentheses or otherwise as convenient) followed immediately by the year of publication in parentheses, as, for example '(Smith, Jones & Robinson, 1970)', or 'Smith, Jones & Robinson (1970)'. Authors' names may be inflected as in 'Smith's (1970) method', but no other separation of name and year is allowable. Names and years must not be juxtaposed in any of these ways unless the intention is to refer readers to further details given in the list at the end of the paper (see below). 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*) 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 предготовлении*) or as having been submitted to or accepted for publication by a particular journal. Dates and spellings of authors' names must be everywhere correct and consistent. At the first mention of a reference the names of all the authors must be given if there are not more than six authors. The abbreviation '*et al.*' may thereafter be used sparingly if there are more than two authors.

At the end of the paper a list giving full details of all references should be appended on a separate sheet. The references should (i) be arranged in alphabetical order of authors' names (ii) include the initials of all authors and (iii) be *triple-spaced.* 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*; 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 Appendix II. Note that inclusive page numbers are to be given. Authors should ensure that the list of references includes all references mentioned in the paper (text, figures, tables, and abstract) and no others. The paper will not be sent to the printer until the list is complete. Accents and diacritical marks should be transcribed from the original sources.

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 (§ 3) should be included in the reference list, even if the reference is not repeated in the body of the paper.

7. Nomenclature

7.1 *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), ...; O(1), O(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, 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.

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. Examples are C(1), C(1^{i}), C(1^{ii}), C(1^{iii}), C(1^{v}), C(1^{vi}), ..., Na(3^{ii}), *etc.* When the asymmetric unit contains only one atom of a chemical species the arabic numeral should be omitted; if distinction of different asymmetric units is required the superscript may be attached directly to the chemical symbol, *e.g.* Nd^{iv}.

Space groups should be designated by the Hermann–Mauguin symbol, for example *Pba*2. The number assigned in *International Tables for X-ray Crystallography* may be added if desired for reference, for example *Pba*2 (No. 32). As a check on the space-group orientation the systematic absences should be given explicitly. 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.

A symbol such as 123 or *hkl* without brackets is understood to be a reflexion, (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 $f = f_0 + f' + if''$.

Authors are reminded that 'lattice' is a mathematical concept with an exact meaning, and should not be used loosely as a synonym for 'structure'. Note that 'centric' and 'acentric' were brought into the crystallographic literature to 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 Bailey *et al.* [*Acta Cryst.* (1977), A**33**, 681–684].

7.2 *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. They 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), A**33**, 681–684].

Chemical nomenclature and formulae should conform to current IUPAC rules; *any* deviations must be explained. Publications containing these rules are listed in *J. Am. Chem. Soc.* (1976), **98**, 8A. The prefixes iso and bis should not be italicized. Chemical formulae should not be used as abbreviations for chemical names unless this results in increased clarity of expression or has the additional object of emphasizing composition or structure.

It is generally desirable to include the chemical formula in the title, abstract or first paragraph of the paper. It should be included in the title or abstract if it is not well known or deducible without ambiguity from the name of the substance. Please see comments under *Typography* concerning displayed formulae (§ 8.3).

7.3 *Units*

The system of metric units known as SI should be used, except that the ångström (symbol Å, defined as 10^{-10} m) is preferred to the nanometer (nm) or picometer (pm). When there is good reason for using other units (for example, when a dimension is determined by a standard machine tool or commercially available material) the metric equivalent should follow in parentheses. Examples: A rod of diameter $\frac{1}{4}$ inch (~6·3 mm). ... A screw with a pitch of 25 threads to the inch (~0·984 threads per mm) ...

7.4 *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 small dictionaries of the language of the paper.

8. Typography

8.1 *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 our printers. Authors should, however, indicate by a wavy underline mathematical symbols or other materials that are to be printed in **bold type.** It is usually unnecessary for authors to indicate *italic* type, but when they desire to do so it should be done by a straight underline. This straight underline is a convenient way of distinguishing the italic letter *l* from the figure 1 when the typewriter has the same face for both, and also for distinguishing letter *O* or *o* from zero. When roman capital O is likely to be confused with zero it may be given a triple underline. For other possibilities of ambiguity see § 8.2.

8.2 *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. Mathematical expressions, whether typed or written by hand, should be presented as nearly as possible in the form in which they are expected to appear in print (for example, all subscripts, superscripts, straight lines separating numerators from denominators, signs of equality, *etc.* should be at the proper levels in relation to each other). Exponential expressions, unless very simple, should be written in the form exp(...). The use of expressions containing subscripts to superscripts or the like should be kept to a minimum. Simple expressions not requiring to be displayed should if possible be written so that they do not need extra space between lines of text, for example $(\sin\theta)/\lambda$ rather than $\frac{\sin\theta}{\lambda}$. The power $\frac{1}{2}$ is preferable to the square-root sign.

Long mathematical formulae should be written so that they can be printed on several lines rather than stretching across the printed page. The solidus or the use of the power -1 is preferable to a long rule in a fraction in which either numerator or denominator or both are longer than a single column width when printed.

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.

Letters or signs that can be confused when handwritten (such as a, d, α; I, I, 1, l; u, n, h, η, μ; x, $\times$, X, χ, κ; v, r, ν, γ; 2, z; ξ, ζ; w, W, ω; E, ε, $\in$) should be very carefully distinguished, if necessary by marginal notes. On no account, however, should Greek letters be underlined, except for a wavy line to indicate bold type. 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, or when Greek letters are spelled out (for example whether 'sigma' means Σ or σ). Where a Greek capital letter is required, this should be stated unless the handwritten capital 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.

8.3 *Chemical and structural formulae*

Some structural formulae cannot be set up in type satisfactorily, and in such cases it is necessary for a block to be made; authors are advised to supply drawings for this purpose. Lettering and numbering can be added by the printers as for diagrams (see §§ 4.4–4.6). Formulae to which these remarks apply include those of ring systems in which the author wishes to demonstrate the actual angles between bonds, formulae containing curved lines, and formulae in which bonds are represented by lines of different or varying thickness.

9. 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.

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 $\frac{1}{2}$%.

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).

When absorption, extinction, or any special corrections or scale factors are applied in the reduction of the intensity data, the method and formulae used should be given.

Additional recommendations concerning the reporting of computations in structure determination, based on material supplied by the Commission on Crystallographic Computing, are contained in Appendix III.

10. Auxiliary publication procedure (deposition)

10.1 *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 in at least two depositories, from one of which a reader can obtain photocopies without charge to him (§ 10.2).

Except as provided in § 5.2, tables of structure factors and of anisotropic thermal parameters are deposited. Other parts of papers that may be appropriate for deposit are the following:

(i) Additional details of the experimental procedure.

(ii) Additional details of the stages of structure refinement.

(iii) Detailed tables of bond lengths and bond angles, especially when of limited accuracy (*e.g.* those involving hydrogen atoms whose parameters have not been thoroughly refined).

(iv) Additional details of mathematical derivations given only in outline in the main text.

(v) Lengthy discussions of points that are not of primary interest, or that do not lead to definite conclusions, but do have significant value.

Authors should indicate clearly those parts of their papers intended for deposit. Acceptance of a paper may be conditional on the deposit of further parts.

10.2 *The procedure*

All material to be deposited is subject to the usual refereeing procedure (§ 11.1).

The International Union of Crystallography will arrange for the deposit of one set in the British Library Lending Division, Boston Spa, England, and of another set elsewhere. Photocopies of the set deposited in the British Library Lending Division may be obtained by readers without charge to themselves on application to the Executive Secretary of the Union. The deposit reference number appearing in the published paper must be quoted in the application. Authors outside the United Kingdom are encouraged to arrange a third deposit in their own country, in addition to the two made by the Union.

10.3 *Preparation of material for deposit*

Two additional copies of the title, name(s) and address(es) of the author(s), and of the abstract are required (all on one page), as well as two copies of the material intended for deposit; authors may find it convenient to provide all this in the form of two additional copies of the complete paper (see § 2.5).

Text and tables to be deposited should be clearly typed with a fresh black ribbon (blue is not acceptable) on pages of normal size, but there is no need to strive for extreme compression of presentation. 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).

Authors will be responsible for the preparation of material according to the following specifications:

(*a*) Optimum page size for text or tables in typescript: up to 30 cm × 21 cm.

(*b*) Limiting page size for text or tables in typescript: 33 cm high × 24 cm wide.

(*c*) Limiting size for diagrams, graphs, spectra, *etc.*: 39 cm × 28·5 cm.

(*d*) Tabular matter should be headed descriptively on the first page, with column headings recurring on each page.

(*e*) Pages should be clearly numbered to ensure the correct sequence.

Structure-factor tables prepared from computer printout must be presented in the form indicated above, not in the form of continuous printout, and must be arranged with the greatest economy of space possible. The printout must be in clear black type and must not be printed on paper with coloured stripes if the legibility of the tables is not to be impaired seriously. A suitable program for producing computer printout in the required page size (30 cm × 21 cm) and including table headings and page numbers is the *CRYSLSQ* program, which is part of the *XRAY* system of programs [*e.g.*, Stewart, Kundell & Baldwin (1972). *The X-RAY System of Crystallographic Programs*. Tech. Rep. TR-192, Computer Science Center, University of Maryland, College Park, Maryland 20740, USA; 1970 and 1976 versions also exist]. All columns must be headed. A 'paste-up' on white card of computer printout will be acceptable provided that the quality of the printout is adequate.

11. Action that follows submission of a manuscript

11.1 *Publication mechanics*

The editor who receives a manuscript (see § 1.2) will acknowledge it, will obtain referee reports as required, and will correspond with authors as necessary regarding acceptance, rejection or revision of the manuscript. When the receiving editor finds the manuscript acceptable in both scientific quality and general form, he so notifies the author(s) and sends the manuscript to the Technical Editor. The Technical Editor checks numerous aspects of format and usage, clarity for the printer, quality of figures for reproduction, *etc.* He sometimes finds it necessary at this point to communicate with the author concerning some technical point about such things as typography, table layout, figure clarity or suitability for reproduction, *etc.* The Technical Editor then marks the manuscript with the necessary instructions to the printer. The printer prepares proofs and sends copies both to the first-named (or otherwise indicated; see § 2.4) author and to the Technical Editor. After making the minimum necessary corrections, the author sends the proofs to the Technical Editor who adds his own corrections and returns one set of fully corrected proofs to the printer for publication.

11.2 *Proofs*

Proofs (2 copies) of papers are sent to the first-named author at the address given in the heading of the paper, *unless other instructions are given at the time of submission, preferably on the typescript.* Corrections should be indicated on the proofs and not (unless there is insufficient space) on separate sheets of paper. Ink or ball-point pen should be used (not green, please; that colour is reserved for the printer) and all markings must be legible and without ambiguity (see also § 8.2). One copy of the proof should be retained by the author, and the other copy should be sent as soon as possible to the Technical Editor. (Serious delay is probable if the proof is returned to anyone other than the Technical Editor.) The Editorial Board reserves the right to make a charge for alterations in proof other than the correction of printers' errors. If such alterations are unavoidable, every effort should be made to substitute words or phrases equal in length to those deleted.

The Journals reserve the right to proceed with publication without benefit of the author's corrections if the author's marked proofs are not received promptly.

11.3 *Offprints (reprints)*

An order form for offprints (reprints) is sent along with proofs and should be returned to the publishers (Munksgaard), *not* to the Technical Editor, at approximately the same time that the proofs are returned to the Technical Editor. Only offprints specifically ordered will be supplied; 25 will be provided free *if ordered.* Further copies, without limit in number, may be purchased at this same time at a price specified on the order form. Except in very special circumstances, the requirements of all authors and their laboratories should be included in a single order. Orders, whether for free or additional offprints, can be filled only if submitted promptly.

11.4 *Return of material*

Typescripts and figures are not normally returned to authors, and may be destroyed after publication of the papers. Authors may request the return of their material or any part of it, such as figures only. Requests for the duplicate copies used for refereeing (§ 2.5) should be included in the letter of submission; request for the return of the copy used by the printer should be addressed to the Technical Editor when the proofs are returned.

APPENDIX I

Categories of contributions

Ordinary articles

Original articles on some aspect of crystallography (see also § 1.1) 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.

Short Structural Papers

Section B of *Acta Crystallographica* publishes short-form structure papers under a special heading. These must be submitted in a prescribed format (Appendix IV); they are refereed in the normal way and printed in the same type size as ordinary articles, but are given priority at all stages of handling. They are not to be regarded as interim reports, but as final accounts.

Short Communications

Short Communications differ from ordinary articles not only in being shorter (see § 2.6), 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.

Reference Information

The *Journal of Applied Crystallography* publishes short contributions of this type when appropriate. These are sent to referees; acceptance and printing can be quicker than for ordinary articles. Among the kinds of information accepted are the following:

(*a*) *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. Such data must be submitted in a prescribed format (Appendix V).

(*b*) Announcements of the availability of crystallographic *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.

(*c*) Announcements of the availability of *Bibliographies* relevant to crystallography.

Comment

Comment is visually distinguished from the other types of contributions by the use of different typography. It appears

only in *Journal of Applied Crystallography*. The material is not sent to referees. Five categories of Comment are accepted at present:

(*a*) *Laboratory Notes*. 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. One figure or photograph may be included if it will be useful when reduced to one-column width in a three-column-per-page style (see § 4.3) and if the total column space does not ordinarily exceed $\frac{1}{2}$ to $\frac{3}{4}$ of a single column (200 to 300 words). Because of this size limitation 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*.

(*b*) *Letters to the Editor*. Selected *Letters to the Editor* are published. They 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.

(*c*) *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, *etc.* It is hoped that all crystallographers will participate as reporters for this section, as the editors alone cannot know more than a very small fraction of the items which should appear. Please send these contributions to the Executive Secretary of the Union.

(*d*) *Meeting reports*. These are normally invited.

(*e*) *Meetings*.The category headed *Forthcoming Meetings and Short Courses* carries listings of interest to crystallographers. These will include meetings of scientific societies, congresses, summer schools, *etc.* The meetings so described and other forthcoming events are summarized in the *Calendar of Events* in each issue. Contributions should be sent to the Executive Secretary of the Union.

APPENDIX II

References

Fig. 1. shows an example of a typescript list of References set out in accordance with § 6.

References

Åsbrink, S. & Magnéli, A. (1959). Acta Cryst. 12, 575-581.

Babel, D. (1972). Z. Anorg. Allg. Chem. 387, 161-178.

Bijvoet, J.M., Peerdeman, A.F. & van Bommel, A.J. (1951). Nature (London), 168, 271-272.

Brown, H.C., McDaniel, D.H. & Häfliger, O. (1955). Determination of Organic Structures by Physical Methods, edited by E.A. Braude & F.C. Nachod, pp.567-662. New York: Academic Press.

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

Fig. 1. Facsimile (actual size) of a specimen list of references, illustrating correct spacing and arrangement.

References (continued)

Derry, J.E. (1973). The Crystal and Molecular Structures of Four Organic Compounds. PhD Thesis, Univ. of Birmingham.

Fritchie, C.J. Jr (1966). Acta Cryst. 20, 892.

Hauptman, H. (1971). Am. Crystallogr. Assoc. Winter Meet., Abstract H3, p.49.

Hauptman, H. (1975). Summer School on Crystallographic Computing, Prague. Published as Crystallographic Computing Techniques (1976), edited by F.R. Ahmed, pp.120-130. Copenhagen; Munksgaard.

McDonald, T.R.R. (1956). Acta Cryst. 9, 162-168.

Machatschki, F. & Mussgnug, F. (1942). Naturwissenschaften, 30, 106.

Pèpe, G. & Pierrot, M. (1972). Acta Cryst. B28, 2118-2123.

Shifrin, K.S. & Perelman, A.Y. (1967). Proc. Second Interdisciplinary Conference on Electromagnetic Scattering, pp.131-167. New York: Gordon & Breach.

Stewart, J.M., Kruger, G.J., Ammon, H.L., Dickinson, C. & Hall, S.R. (1972). The XRAY System - version of June 1972. Tech.Rep. TR-192. Computer Science Center, Univ. of Maryland, College Park, Maryland.

Fig. 1 (*cont.*)

References (continued)

Tamure, C. (1971). Yuki Gosei Kagaku Kyokai Shi (J. Synth. Org. Chem. Jpn, in Japanese), 29, 977-990.

Van der Helm, D., Ealick, S.E. & Burks, J.E. (1975). Acta Cryst. B31, 1013-1018.

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

IUPAC-IUB Commission on Biochemical Nomenclature (1970). J. Mol. Biol. 52, 1-17.

Karle, I.L. (1970a). Acta Cryst. B26, 765-770.

Karle, I.L. (1970b). Acta Cryst. B26, 1639-1645.

Karle, I.L. & Karle, J. (1950). J. Chem. Phys. 18, 957-962, 963-971.

Karle, J. (1966). Acta Cryst. 21, 273-276.

Kelstrup, E. & Kjaer, A. (1975). Chem. Commun. pp.629-630

Kojić-Prodić, B., Deanović, A. & Brničević, N. (1976). J. Appl. Cryst. 9, 485-490.

Konnert, J.H. & Karle, J. (1973). Acta Cryst. A29, 702-710; erratum (1974), A30, 679.

Fig. 1 (*cont.*)

References (continued)

Laue, M. von (1960). Röntgenstrahlinterferenzen, 3rd ed., p.467. Frankfurt am Main: Akademische Verlagsges.

Le Marouille, J.Y. (1972). Thèse de Doctorat de 3e Cycle, Rennes.

Fig. 1 (*cont.*)

APPENDIX III

Computing details

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 reflexions given zero weight).

When information about crystal shape and orientation was needed for absorption or extinction corrections, this information should be given in sufficient detail for the reconstruction of the actual ray paths.

A final agreement index or residual, R, based on all measured reflexions, should be defined and quoted. The treatment of multiplicities, of reflexions measured as zero or negative, and of reflexions 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.

Formal estimated standard deviations (e.s.d.'s) should be quoted and their basis defined.

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.

All computer programs used in the crystallographic analysis should be identified both in the text and in the reference list, as specified in § 6.

APPENDIX IV

Short Structural Papers

A paper submitted for consideration as a Short Structural Paper must not exceed three printed pages of *Acta Crystallographica* (about eight pages of manuscript; text, figures and tables to be printed all being counted in this total), and must conform to the following scheme:

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

The *Abstract* will consist (preferably in the order given here) of the formula, crystal system, space group, unit-cell dimensions with an indication of accuracy (normally the standard deviation in units of the last quoted decimal place enclosed in parentheses), cell content, measured and calculated density, source of the material, and such other information (especially structural) as can be conveyed in approximately 50 further words.

The *Introduction* will state the reason for undertaking the structure determination and its chemical or physical interest, the methods of data collection and of structure determination (if either method is novel and requires detailed description a short format should not be used), give the systematic absences (if any) and other space-group evidence explicitly, cite the number of reflexions measured (including the number of those measured as zero) and the number of those accessible in principle but not actually measured, and give at least the residual based on all measured reflexions (including those measured as zero); other residuals may be given if the author desires. Environmental circumstances if relevant (unusual temperature or pressure; actual room temperature if the accuracy of the cell dimensions is high) should appear in the abstract. Crystal size and absorption coefficient should be given whenever relevant.

The *atomic coordinates* and the *thermal parameters* should be presented in tables. An indication of accuracy (preferably the standard deviation in units of the last significant figure) should be given. The table of coordinates will be published; the table of thermal parameters will normally be deposited, and should conform to the requirements of the deposition scheme (§ 10.3).

Bond lengths and *bond angles* should be indicated on a figure if possible, or (within the original limit of length of a Short Structural Paper) in a table. If they are very numerous they should be presented in a table suitable for deposit (§ 10.3), and the unusual ones (if any) mentioned in the *Discussion*.

The *Discussion* will comment on any unusual features of coordination, bonding, bond lengths and bond angles.

Any non-routine measurement of *physical properties* (magnetic susceptibility, dielectric constant, 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 immediately preceding *Discussion*.

Structure-factor tables (observed and calculated) must be submitted in duplicate with the paper, but will not normally be published. After acceptance of the paper they will be deposited, along with any other extensive tables, in accordance with the Union's procedure (§ 10). If, for good reason, the tables are intended for publication with the paper, they should instead conform to normal requirements (§ 5.3) of suitability for direct photographic reproduction with a density of at least 2000 per page.

The requirements regarding *figures* and *references* are the same as in the case of ordinary articles. Acknowledgments may be included at the end of the text.

APPENDIX V

Format for 'Crystal Data'

Contributions for the section *Crystal Data* of *Journal of Applied Crystallography* 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.]

Abstract

Give quantitative results, such as lattice parameters, space group, and specific compound identity not already conveyed by the title, and indicate what additional data, such as powder data, are given.

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 (oriented Hermann–Mauguin symbol) if determined.

State diffraction method with radiation and numerical value used for the wavelength. List cell data (with temperature of observation if required by stated accuracy) with the standard deviation given in parentheses, in units of the last digit of the cited value, in the format:

$a =$ ( ); $b =$ ( ); $c =$ ( ) Å;
$\alpha =$ ( )°; $\beta =$ ( )°; $\gamma =$ ( )°;
$U =$ Å^3; $Z =$;
$D_m =$ ( ); $D_x =$ g cm^{-3} [or the SI unit Mg m^{-3} may be used].

Powder data

State radiation and numerical value used for the wavelength, type of instruments used (*e.g.* standard diffractometer, HDS camera, Guinier camera, *etc.*) method of intensity determination and any special features of the diffraction geometry of apparatus. Tabulate data under the headings

$$d_{obs} \quad d_{calc} \quad hkl \quad I/I_0$$

Intensities are taken to be peak intensities unless otherwise stated.

Crystal morphology

List here 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 here the data determined for physical properties such as:

Optical properties: indices, measured 2V, 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, resonance spectra (infrared, n.m.r., *etc.*)
Diaphaneity, colour, streak, lustre, hardness, *etc.*
Other physical properties.

Comparison with other results

State succinctly whatever can usefully be said.

For further suggestions, see Kennard, Speakman & Donnay, *'Primary Crystallographic Data,'* [*Acta Cryst.* (1967), **22**, 445–449], Kennard, Hanawalt, Wilson, de Wolff & Frank-Kamenetsky, *Powder Data* [*J. Appl. Cryst.* (1971), **4**, 81–86].

APPENDIX VI

Check list for authors, referees and editors of crystal structure papers

This check list* is provided to assist authors in ensuring that they have provided information sufficient for critical appraisal of their results. It is not necessarily complete nor is it necessarily mandatory that each item listed be provided in every paper; it is recognized that the nature and range of detail required does vary with the purpose and intended precision of the structure analysis. Presentation of the information should always be concise, and in the short format (Appendix IV) whenever possible.

A. Abstract. In addition to the physical or chemical features of importance, the abstract should contain:

1. Chemical formula and name, unless included in the title.

* Based on recommendations originally provided by the Committee on Chemical Crystallography of the [US] National Academy of Sciences – National Research Council; modified to reflect the current practice of *Acta Crystallographica*.

2. Lattice parameters and standard deviations; crystal system; space group (Hermann–Mauguin symbol); number of formulae per unit cell (Z).
3. Intensity-measurement method used.
4. Refinement method; specify R and give final value.
5. Brief description of overall structure, including bond lengths and angles of major interest.

B. Experimental. This section should permit replication of the experiment by others and contain:

1. Method of establishing chemical formula; source of material; crystal colour; habit.
2. Lattice-parameter measurement method(s), temperature(s), radiation(s) and wavelength value(s) used. If different, lattice parameters of standard cell and transformation matrix to cell used.
3. Z; X-ray density; measured density; method of density measurement.
4. Laue symmetry, systematic absences: possible space group(s); tests for centre of symmetry; general equivalent positions if unconventional setting (*i.e.* not that of *International Tables for X-ray Crystallography*).
5. Crystal dimensions and orientation with respect to crystal axes and camera or diffractometer axes; μ; absorption-correction method; maximum and minimum absorption corrections.
6. Intensity measurement:
   (*a*) Radiation and detector used; measures taken to exclude unwanted wavelengths.
   (*b*) If film: method used to measure intensities; method of scaling intensities between films.
   (*c*) If diffractometer: type of geometry; detector and operating conditions; derivation of integrated intensity from measurements; corrections for TDS, white radiation, *etc.*
   (*d*) Measure of agreement among equivalent reflexions.
   (*e*) Method of assigning standard deviations of intensities.
   (*f*) Definition of unobserved reflexions; handling of 'below threshold' intensities.
   (*g*) Number of reflexions measured; number of independent reflexions; (sin θ)/λ range within which reflexions were systematically measured; total number of reflexions accessible in this range.