International Union of Crystallography

Notes for Authors

Acta Crystallographica, an international journal belonging to the International Union of Crystallography, is published in yearly volumes of 12 issues. Papers are accepted in English, French, German and Russian on all branches of crystallography, including new crystallographic apparatus. Papers on those parts of physics and chemistry which have a structural basis or crystallographic application are also accepted. The submission of a paper is understood to imply that the material is original, that it has not been previously published, and that it is not intended to publish it elsewhere in any language. Besides the results of original research, occasional review articles are accepted. Interim accounts are discussed at the end of these notes.

Articles in English should be submitted to the most convenient of the following Editors: H. LIPSON, R. E. MARSH, S. MIYAKE, D. P. SHOEMAKER. Articles in French should be submitted to J. WYART, in German to H. JAGODZINSKI, and in Russian to A. J. C. WILSON.

Authors are requested to give particular attention to the following points:

Manuscripts. Papers should be in the form of widely spaced (lines at least 8 mm centre to centre) single-sided typescripts (top copies) on good quality paper, and should conform to the general editorial style of the journal. Clarity for the printer, rather than elegance, is the important factor: unconventional usages or possible ambiguities (for example zero or letter *O*, especially when subscript; indices *hkl* or *hk*1) should be explained in marginal notes. Badly prepared typescripts involve much editorial work and are likely to suffer delay in publication. Wide spacing of the lines of typescript is important, since it is necessary to leave room for editorial corrections and rearrangements; it is particularly important to provide plenty of space in the lists of references.

Every manuscript should bear an address sufficient for postal purposes.

It is possible to give quicker consideration to manuscripts that are submitted in duplicate, but submission in duplicate is not required. The manuscript will not be returned with the proofs; authors should therefore retain an exact copy.

The quantity of material submitted for publication is such that the utmost brevity of presentation is essential. Delay and editorial correspondence are avoided if authors check repeatedly whether their presentation can be simplified or abbreviated without loss of essential detail. Only exceptionally can papers be considered which exceed the equivalent of about 6000 words. The primary consideration, however, is one of density of information: often the information contained in several related short papers could have been presented more concisely in a single longer paper. Articles intended for publication as Short Communications should not exceed the equivalent of about 1000 words.

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.

When it is necessary to distinguish crystallographically equivalent atoms in different asymmetric units the distinction should be made by primes superscript to the arabic numeral; if the number of primes exceeds three the continuation should be by superscript small roman figures. Examples are C(1), C(1′), C(1″), C(1‴), C(1^{iv}), C(1^{v}), C(1^{vi}), ..., Na(3″), *etc.*

When the asymmetric unit contains only one atom of a chemical species the arabic numeral may be omitted, and if distinction of different asymmetric units be required the superscript may be attached directly to the chemical symbol.

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). The Schoenflies symbols (for example C_{2v}^{8}) are discouraged. As a check on the space-group orientation the systematic absences should be given explicitly.

A symbol such as 123 or *hkl* without brackets is understood to be an X-ray reflexion, (123) or (*hkl*) a plane or set of planes, [123] or [*uvw*] a direction, and {*hkl*} a form. Other bracket notations should be explicitly defined by the author.

Authors are reminded that 'lattice' is a mathematical concept with an exact meaning, and should not be used loosely as a synonym for 'structure'.

Abstract. Each paper, whether in English or another language, should be preceded by an abstract in English of not more than about 200 words; this abstract should be suitable for reproduction by abstracting journals without change of wording, and should therefore make no reference to tables, diagrams or formulae contained in the paper. The *Guide for the preparation and publication of synopses*, published by UNESCO, is accepted by the International Union of Crystallography as a basis for its abstracts. Copies are provided by the Co-editors on request.

No abstract is accepted for Short Communications.

An author in an Italian-, Spanish-, or Portuguese-speaking country may in addition give a brief summary in the appropriate language at the end of the paper.

Diagrams. Diagrams should be carefully drawn in black ink with the lettering indicated in soft pencil only. The lettering should be kept to a minimum, and lengthy descriptive matter should be embodied in the legend rather than in the figure. Whenever possible, related diagrams (for example, several electron-density projections of the same structure, or electron-density projections and their keys) should be grouped to form a single figure, as this leads to considerable economy in printing;

in any case, such diagrams should be prepared on the same scale and in a uniform style. Fine-scale details should be avoided as far as practicable, and care should be taken that arrowheads, broken lines, and similar small features are sufficiently bold. Examination of drawings through a reducing lens is of assistance in judging whether a diagram is suitable for reproduction. Good quality reduced photographic copies of diagrams are perfectly satisfactory for block making and are easier to handle than original drawings.

Very large drawings give great difficulties to the printers, and even when supplied in cardboard rolls they are likely to be damaged in the post or during editorial procedures. The dimensions of photographs or original drawings submitted should not be more than about twice those intended for the finished diagrams. It is often convenient to make them approximately the same size as the paper on which the manuscript is typed (about $8\frac{1}{2}'' \times 11''$ or 22 cm × 28 cm). Additional copies for submission to referees are helpful.

Photographs intended for half-tone reproduction must be in the form of highly glazed prints. Plates on coated paper are expensive, and authors may be asked to contribute to the cost. Plates in colour are accepted only if the entire cost is paid by the author or his organization.

Every figure should have a legend and these legends should be collected together on a separate sheet.

Tables. Every table must be provided with a caption. Tables of F values, unless very short, can be accepted for publication only if they are presented in a form suitable for direct photographic reproduction. For this purpose they should be very carefully and clearly typed with a dense black ribbon, and should be designed to conform to the shape and dimensions of a page of *Acta Crystallographica* after a linear reduction of 2:1 or $2\frac{1}{2}$:1. Any symbols inserted by hand should be in black ink. The tables should be typed in single spacing (not double spacing, as required for manuscripts) with columns as close together as is reasonably practicable. Special care should be taken that there are no errors and that the columns are properly aligned. An example of a well-designed table will be found in *Acta Cryst.* (1962), **15**, 313. Large tables should be reduced photographically before submission to a size that can be handled without risk of damage, as recommended in the paragraph concerning diagrams.

Mathematics. The printing of mathematics is very expensive, and mathematical arguments should be abbreviated as far as is practicable without loss of clarity. Mathematical expressions should generally be written clearly and carefully in ink, unless a special typewriter is available. Easily confused symbols (such as u, n, h; χ, x, κ; v, r, ν) must be clearly distinguished. Gothic letters should be avoided if possible; if used they should be explained in the margin or elsewhere. Bold-face characters should be indicated by a wavy underline.

Chemical compounds and minerals. The nomenclature of chemical compounds and minerals is not always unambiguous to readers in all countries. Authors are required therefore to quote the chemical formulae, including organic structural formulae when appropriate, of the substances with which their papers deal, and should whenever possible give details of the origin, heat treatment, purity, and experimental density. The temperature at which the measurements are made is often relevant, and should always be quoted in work with any claim to accuracy. It may often be necessary to give the atomic weights of isotopes.

It is generally desirable to include the chemical formulae in the abstract and in the first paragraph of the paper.

References. References should be typed on a separate sheet in the style used in *Acta Crystallographica*, and arranged in alphabetical order of authors' names. Care should be taken that dates and the spellings of authors' names are everywhere consistent, and that authors' initials are given in the bibliography. The abbreviation '*et al.*' should be used sparingly, and *never* at the first mention of a paper.

The following is a specimen reference list:

COHEN, M. U. (1935). *Rev. Sci. Instrum.* **6**, 68.

DE QUERVAIN, M. (1944). *Helv. Phys. Acta*, **17**, 509.

DESHPANDE, V. T. & MUDHOLKER, V. M. (1960). *Acta Cryst.* **13**, 483.

DESHPANDE, V. T. & SIRDESHMUKH, D. B. (1961*a*). *Acta Cryst.* **14**, 353.

DESHPANDE, V. T. & SIRDESHMUKH, D. B. (1961*b*). *Acta Cryst.* **14**, 355.

FRAZER, B. C. (1948). Thesis, Alabama Polytechnic Institute.

HUNTINGTON, H. B. (1958). *Solid State Physics*, **7**, 213.

JETTE, E. R. & FOOTE, F. (1935). *J. Chem. Phys.* **3**, 605.

JOEL, N. & WOOSTER, W. A. (1960). *Acta Cryst.* **13**, 516.

KÄNZIG, W. (1957). *Solid State Physics*, **4**, 150.

KEELING, R. O. & PEPINSKY, R. (1955). *Z. Kristallogr.* **106**, 236.

LIVINGSTONE, R. (1957). *Physico Chemical Experiments*, p. 35. New York: Macmillan.

MAGYAR, H. (1948). *Anz. Öst. Akad. Wiss.* **85**, (12), 166.

MASON, W. P. (1946). *Phys. Rev.* **69**, 173.

MEGAW, H. (1957). *Ferroelectricity in Crystals*, p. 45. London: Methuen.

TENZER, L., FRAZER, B. C. & PEPINSKY, R. (1958). *Acta Cryst.* **11**, 505.

UBBELOHDE, A. R. & WOODWARD, I. (1947). *Proc. Roy. Soc.* A, **188**, 358.

UEDA, R. (1948). *J. Phys. Soc., Japan*, **3**, 328.

WELLS, A. F. (1950). *Structural Inorganic Chemistry*, p. 70. Oxford: Clarendon Press.

Computing details. Sufficient information should be given to permit the calculations to be repeated, or, if need be, extended at any subsequent date by other workers.

The wavelength or lattice parameter used as a standard for measurements of cell dimensions should be stated explicitly if the accuracy claimed or implied is better than $\frac{1}{2}$ %.

A table of numerical values of F_o and F_c should always accompany a structural paper submitted for publication. It should preferably be published with the paper, but otherwise deposited in a public depository (such as the Library of Congress).

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 and the quantity

minimized in least-squares calculations should be specified (including a statement of any reflexions given zero weight).

The computational procedures should be described in sufficient detail to permit independent evaluation of the correctness and reliability of the structure analysis.

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.

A final agreement index, or reliability factor (R index) should be quoted, and defined with respect to the treatment of the unobserved reflexions and multiplicities.

The correctness of the final structure should be checked, if possible, by a method independent of the refinement procedure. Thus, least-squares or differential-synthesis methods of refinement should be verified by difference-Fourier syntheses to ensure that no important parameters have been overlooked.

Formal estimated standard deviations (e.s.d.'s) should be quoted and their basis defined. The significance of these e.s.d.'s should be discussed in relation to the computational procedures employed (*e.g.* diagonal *versus* non-diagonal least squares, convergence-acceleration methods, weighting scheme, finite-series errors and anharmonicity).

The degree of completeness of the refinement calculations should be indicated, for example by giving 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 parameters before and after correction should be given.

All computer programs used in the crystallographic analysis should be identified, when possible, by publication references to the author of the program in the body of the text.

Proofs. Unless other instructions are given *on the typescript*, proofs of papers will be sent to the first-named author. They should be returned to the Technical Editor (*not* to the publishers) after correction. 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.

When reading proofs, authors should check that all references are complete, as any omission will delay publication.

An order form for reprints is sent out with the proofs, and should be returned to the publishers (*not* to the Technical Editor). Only reprints specifically ordered will be supplied; twenty-five will be provided free *if ordered*. Further copies, without limit in number, may be purchased at a price notified 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 reprints, can only be carried out if submitted promptly.

In order to reduce publication delays, proofs of Short Communications will be read by the Technical Editor, and will be sent to the authors only if they present special difficulties. Order forms for reprints will be sent to the authors in the same way as for papers.

Interim reports on work in progress. The primary purpose of *Acta Crystallographica* is to publish final accounts of original research, and it has never been the intention of the Editorial Board that interim accounts of work in progress should appear in the section 'Short Communications'. 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.

Short Communications drawing attention to the crystallographic aspects of work published in detail elsewhere will be considered on their merits, but cannot be given high priority in publication.

Book Reviews

Works intended for notice in this column should be sent direct to the Editor (A. J. C. Wilson, Department of Physics, University College, Cathays Park, Cardiff, Great Britain). As far as practicable books will be reviewed in a country different from that of publication.

The art and science of growing crystals. Edited by J. J. Gilman. 493 pp. New York and London: John Wiley & Sons. Inc., 1963. Price £7.10*s*.

Es ist überflüssig, hier zu betonen, welche hervorragende Bedeutung heute die Kristallzüchtung in Wissenschaft und Technik erlangt hat. Die Anwendung synthetischer Kristalle (als Oszillatoren, Polarisatoren, Kristallzähler, optische Medien, Halbleiter, Piezoelektrika, Maser, Laser usw.) hat in den letzten 15 Jahren eine ungewöhnlich intensive und extensive Entwicklung erfahren, und doch scheint es so, als stünde dieser Trend noch am Beginn. In einer solchen Phase der Ausweitung einer wissenschaftlich-technischen Disziplin ist es immer nützlich, die praktischen Fragestellungen mit ihren theoretischen und experimentellen Grundlagen unmittelbar zu konfrontieren. Das ist das wesentliche Anliegen der Monographie *The art and science of growing crystals*, die mit grosser Sachkenntnis von Prof. J. J. Gilman herausgegeben wurde. Der Grundgedanke ist die unmittelbare Verknüpfung der 'Kristallzüchtung' mit den wissenschaftlichen Prinzipien der Keimbildung und des Kristallwachstums.

Das Buch gliedert sich in vier Hauptteile: Wachstum aus der Dampfphase, Kristallisation aus Lösungen und Präzipitationen bei Reaktionen, Wachstum aus der Schmelze und Rekristallisation. Jeder dieser Hauptteile wird mit einem allgemein grundlegenden Artikel eröffent: Theorie des Kristallwachstums aus der Dampfphase (N. Cabrera, R. V. Coleman), allgemeine Grundlagen der