Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. The notes (in duplicate) should be sent to the Executive Secretary of the International Union of Crystallography (J. N. King, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England).

Duplicate publication of papers

As stated in *Notes for Authors* (this issue, p. 97, paragraph 1.3), it is not the policy of *Acta Crystallographica* to publish material that has already appeared, or is intended to appear in any other journal in any language. A paper showing a significant advance on results published in preliminary form will be considered by the Editors; authors of such papers are requested to provide copies of the preliminary note along with the paper intended for publication. Papers showing only a marginal advance on the earlier publication will be rejected.

This reminder is considered desirable at this time, as there has recently been an increase in the submission of papers duplicating material already published and the Editors have not always recognized the duplication. It does not mark a change in editorial policy; essentially the same condition has appeared in earlier *Notes for Authors* [see, for example, *Acta Cryst.* (1965), **18**, 134 (first paragraph)].

International Union of Crystallography

Acta Crystallographica
Journal of Applied Crystallography

Airfreighting of copies to the U.S.A. and Canada

As from 1 January 1973 all deliveries of *Acta Crystallographica* and *Journal of Applied Crystallography* to the U.S.A. and Canada will be by air freight to New York and thence by second class mail. This is expected to save about four weeks in delivery times. To cover the cost of this improved service it will be necessary to make annual charges which will be additional to the usual subscription and will be obligatory for all subscribers in the U.S.A. and Canada. These additional charges are as follows

Acta Crystallographica

Sections A & B (combined subscription)	Add D.kr.70	($10·50)
Section A only	Add D.kr.20	($ 3·00)
Section B only	Add D.kr.50	($ 7·50)

Journal of Applied Crystallography Add D.kr.20 ($ 3·00)

These charges are fixed in Danish kroner. The U.S. dollar equivalents are subject to exchange rate fluctuations.

Acta Crystallographica

The Executive Committee of the International Union of Crystallography has found it necessary to announce increases in the yearly subscription rates for to *Acta Crystallographica* as from 1 January 1973. The following rates will apply for Volumes A29 and B29 (1973).

Complete volumes, regular price per volume

Sections A & B (combined subscription)	D.kr.1100	($161·00)
Section A only	D.kr. 250	($ 36·50)
Section B only	D.kr. 950	($139·00)

Complete volumes, reduced price for individuals

Sections A & B (combined subscription)	D.kr. 440	($ 64·40)
Section A only	D.kr. 100	($ 14·60)
Section B only	D.kr. 380	($ 55·50)

All subscription rates are fixed in Danish kroner, and the U.S. dollar equivalents are subject to exchange rate fluctuations. All subscribers in the U.S.A. and Canada should add to the above subscription rates the charges for airfreighting stated in the preceding section. Subscribers to Section A only should note that there has been no increase in their basic rate in Danish kroner.

The yearly subscriptions for individuals are, as heretofore, 40% of the regular subscriptions. These reduced rate subscriptions are ordinarily only available to members of recognized scientific societies, who must give a written undertaking accompanying their subscription application that the journal is for their personal use and will not be made available to libraries, institutions, *etc.*

Journal of Applied Crystallography

The prices in Danish kroner for *Journal of Applied Crystallography* remain unaltered. However, all subscribers in the U.S.A. and Canada should add to the usual subscription rate the additional charge of D.kr.20 for airfreighting as mentioned in the first section above.

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 applications 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, and not to the Technical Editor, who deals with manuscripts only after they have been accepted by one of the editors. Contributions in French should be submitted to an editor with an address in France and contributions in German to an editor with an address in Germany. Contributions in English may be submitted to the Editor or any of the Co-editors. Contributions in Russian may be submitted to an editor with an address in the U.S.S.R. or to the Editor of the journal.

1.3 *Sole publication warranty*

The submission of a paper is understood to imply that the material is original, that it has not been previously published in any language, and that it is not intended to be published elsewhere in any language. The copyright of papers accepted is vested in the International Union of Crystallography, except as otherwise required by national laws.

1.4 *Preparation and handling*

The editor to whom a paper is submitted is responsible 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 connexion 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 which is being recommended by another group.

2. *Typescripts*

2.1 *Paper, margins, spacing, general style*

Contributions should be typed on good quality paper of normal size, should (except as indicated in § 5) be double-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). 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 up 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 *hk*1 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 should be sent. In the absence of other instructions *on 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*

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

2.6 *Manuscript length*

The utmost 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.

3. *Abstract*

Each contribution subject to refereeing (ordinary articles, Short Structural Papers, Short Communications, reference information in *Journal of Applied Crystallography*) must be preceded by an abstract in English. An author whose national language can be printed in Roman or Cyrillic characters but is not one of the usual languages of publication (see § 1.2) may, in addition, give a brief summary in that language at the end of the paper.

Ordinarily 200 words suffice for the abstract for a full paper and 100 for shorter contributions. This abstract should be suitable for reproduction by abstracting services without change of wording. It should, therefore, state as specifically and as quantitatively as possible the principal results obtained. It should make no reference to tables, diagrams or formulae contained in the paper. Similarly, any necessary literature citations should be given in full within the abstract, *e.g.* [Cohen, M. U. (1935). *Rev. Sci. Instrum.* **6**, 68–79], but the inclusion of literature citations should be avoided if possible.

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 *Quality, backing, colour*

Diagrams must be provided in 'hard copy' form, that is, as carefully made original drawings in black ink or high-quality photographic copies (glazed prints). Diagrams should not be submitted on fragile material (such as some types of tracing paper and tracing plastic) or in unnecessarily large size.

If they meet the other requirements, good quality reduced photographic copies of diagrams are perfectly satisfactory and are easier to handle than original drawings, especially when the latter are very large (see § 4.2).

Photographs intended for half-tone reproduction must be in the form of highly glazed prints. The general requirements stated below for diagrams apply also to photographs. 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.

4.2 *Size*

Diagrams should be designed in the knowledge that they will be reduced to the smallest size consistent with clarity, 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; on account of their large size they may give difficulties to the printers and are likely to be damaged during handling or in the post, particularly if packed in rolls.

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

Diagrams intended for stereoscopic viewing should be submitted on the correct scale with approximately 55 mm between centres, ready to be published without size reduction or change of separation.

4.3 *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 finally printed form, is reasonably consistent with the style of the journals, 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 capitals. 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.

4.4 *Lettering and symbols – size and placement*

Fine-scale details and lettering must be large enough to be clearly legible after the whole diagram has been reduced to a convenient size. 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 – 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 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*).

4.6 *Numbering and legends*

Diagrams and photographs should be numbered as Figures in a single series, normally in the order in which they are referred to in the text, but some departure from this order may be permitted to allow a number of half-tone photographs to be printed on a single sheet of art paper. Every figure without exception must have a legend to be printed below it with the Figure number. A list of the legends ('Figure captions') should be attached to the manuscript. In both the list and in the text, the abbreviation 'Fig.' is used when figures are identified by number.

4.7 *Number of copies*

Additional copies of Figures for sending to referees are helpful; they reduce the risk of damage to the originals.

5. *Tables*

5.1 *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. For reasons of economy, small tables will usually be set in type and only very large tables will be photographed.

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, thermal and positional parameters should be prepared in such a way that they do not require the printing of large numbers of zeros. Tables which appear to be wasteful of space will be returned to the authors for reconstruction, with consequent delay in publication.

To avoid damage and difficulties in handling, very large tables should be reduced photographically to a convenient size before submission. Authors should check that the prints submitted are clearly legible in every part and are free from errors, ready for photographic reproduction. To avoid delay and the expense of another printer's block, the Technical Editor may use a footnote to draw attention to errors detected in proof. Tables to be photographed should be typed in single spacing. The editors will return to the author for modification any Table that in their view has too much space between lines.

5.2 *Structure-factor tables*

Structure-factor tables will either be published with the rest of the paper or be deposited in accordance with the auxiliary publication scheme (§ 10). The decision is made by the Editor or Co-editor after consultation with the authors and referees.

5.2.1 Structure-factor tables to be published with the paper are reproduced photographically. 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.

An example of a well-designed F table will be found in *Acta Cryst.* (1971), **B27**, 1796–1799.

5.2.2 Structure-factor tables to be deposited under the auxiliary publication scheme must conform with the requirements of that scheme (§ 10.3). In view of the difference in requirements between tables for publication and tables for deposit, it is suggested that authors may wish to consult the Editor or Co-editor informally before preparing the tables in final form.

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. 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. If two separate references by exactly the same author or authors were published in the same year, they are distinguished by adding the letters, *a*, *b*, to the dates. 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 triply spaced. Names of journals should be abbreviated as they are in the *World List of Scientific Periodicals*. References to books should give the full title, 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 text; the paper will not be sent to the printer until the list is complete. Accents and diacritical marks should be carefully transcribed from the original sources. Proposed publications may be described as 'in the press' (*sous presse, im Druck, в печати*)* if they have reached the printers. Otherwise they may be described as 'in preparation' (*en préparation, in Vorbereitung, в предегомовлении*) or as having been submitted to or accepted for publication by a particular journal.

The abstract will not normally contain references. (See § 3 for instructions on handling the exceptions.)

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^{iv}), 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). Use of the Schoenflies symbols (for example C_{2v}^8) is discouraged. 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.

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.

Authors are reminded that 'lattice' is a mathematical concept with an exact meaning, and should not be used loosely as a synonym for 'structure'. The terms 'centric', 'acentric', which may be applied to intensity distributions, should not be used to describe space groups where 'centrosymmetric', 'non-centrosymmetric' are meant. The proper names Fourier and Patterson should not be used as common nouns, nor

should *e.g.* an electron-density projection be described as a 'Fourier projection'.

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 when appropriate, 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.

Care should be taken to avoid ambiguities in describing certain solvents. For example, amyl alcohol is not identical with normal pentanol, but is a mixture of isomers of the latter. Low-boiling petroleum fractions should be described as light petroleum or petroleum spirit (give the boiling range if necessary) and not as 'petroleum ether'. In recording concentrations of the common mineral acids or mixtures thereof it should be borne in mind that the ordinary 'concentrated' acids are not 100%.

Chemical nomenclature and formulae should conform to IUPAC rules and to the usage of the major chemical journals. Obsolete nomenclature should be avoided. Authors are reminded that the prefixes iso, bis, and n- (for normal) 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, but a structural formula should not be displayed if the chemical structure can be indicated by a formula which can be printed on one line. Please see, also, 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 $\frac{1}{4}$ in. (~6·3 mm)...; A screw with a pitch of 25 threads to the inch (~0·984 threads per mm)...

7.4 *Abbreviations*

Unless they can be looked up in an ordinary translingual dictionary or are commonly used and known by nearly all crystallographers, abbreviations should be explained in the text where they first appear.

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 any 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 on *Mathematics and letter symbols.*

The above-mentioned conventions for indicating italic and bold type should be strictly adhered to, notwithstanding the existence of so-called standards in which the uses of the two kinds of underline are interchanged. Such standards are not commonly acceptable to printers and are in any case unsuitable for material in which italicized symbols are more numerous than those in bold type.

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 $\frac{\sin\theta}{\lambda}$.

Letters or signs that can be confused when handwritten (such as *a*, *d*, α; *u*, *n*, *h*, η, μ; *x*, $\times$, *X*, χ, κ; *v*, *r*, ν, γ; 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, S, U, X, Z, or when Greek letters are spelled out (for example whether 'sigma' means $\sum$ 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 connexion 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 §§ 4.1–4.5). 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, 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 $\frac{1}{2}$%.

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). It should be in the form described in § 5.2.1 if it is to be published with the paper. If it is not published with the paper, it will be deposited in at least two depositories of national or international scope, from at least one of which requesters can obtain copies without charge.

Authors may also, if they wish, deposit additional voluminous experimental details and discussion of results (see § 10).

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.

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

Detailed 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 scheme*

10.1 *Purpose and scope of scheme*

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).

Among the 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) Structure-factor tables, unless they form a critical part of the paper.

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

(v) Lengthy discussions of points which are not of primary interest, or do not lead to precise conclusions.

The decision about which parts (if any) of a paper are to be deposited is made by the Editor or Co-editor after consultation with the author(s) and referees.

10.2 *Procedure*

All material to be deposited is subject to the usual refereeing procedure (§ 11.1). Two additional copies of the title, name(s) and address(es) of the author(s), and of the abstract are required, 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 (*i.e.* three copies of the paper in all). The International Union of Crystallography will arrange for the deposit of one set in the National Lending Library, Boston Spa, England, and of another set elsewhere. Photocopies of the set deposited in the National Lending Library may be obtained by readers without charge to themselves on application to the Executive Secretary of the Union. The reference number mentioned in the published paper must be quoted in the application. Full details are given in the announcement on page 1975 of *Acta Crystallographica*, vol. B28 (1972), and are repeated from time to time among the advertisement pages of the journals.

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 *Form of tables for deposit*

Tables to be deposited under the auxiliary publication scheme should be clearly typed with a fresh black ribbon (blue is not acceptable) on pages of normal size (A4, 8 inch by 10 inch, $8\frac{1}{2}$ inch by 11 inch, or similar), 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. Clear computer output, cut and pasted to form pages of normal size if necessary, is acceptable if on plain (unlined) paper.

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 the 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 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 should be used, 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 editors reserve the right to publish articles with only the Technical Editor's corrections if proofs are not returned promptly.

11.3 *Reprints*

An order form for reprints is sent along with the 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 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 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 reprints, can only be carried out if submitted promptly.

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 in being shorter (see § 2.6), 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 under the heading *Reference Information* when appropriate. These are sent to referees; acceptance and printing are usually quick. Among the kinds of information accepted are the following:

(*a*) Announcements of the availability of bibliographies relevant to to crystallography.

(*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 ordinarily, also, 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*) *Crystal data.* Both powder data and single-crystal data of well characterized materials are accepted. Such data must be submitted in a prescribed format (Appendix V).

Comment

Comment is visually distinguished from the other types of contribution by the use of different typography. It appears only in *Journal of Applied Crystallography*, and 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 § 4.2) 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 paragraph forms an abstract of the whole note.

(*b*) *Letters to the Editor.* Selected letters to the Editor are published, dealing with non-technical aspects of crystallography, its role, its propagation, the proper functions of its Societies, *etc.*

(*c*) *Crystallographers.* The category headed *Crystallographers* 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.

(*d*) *Meeting reports.*

(*e*) *Meetings.* The category headed *Meetings* carries listings of interest to crystallographers. These will include meetings of scientific societies, congresses, summer schools, *etc.* The editors hope that the crystallographic community will help to keep them informed of the meetings that should appear in this listing.

'Letters to the Editor' should be sent to the Editor only; items in other categories of Comment may be sent to any Co-editor.

APPENDIX II

References

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

References

AMMON, H.L., WATTS, P.H. & STEWART, J.M. (1970). Acta Cryst. B26, 1079-1088.

AMMON, H.L., WATTS, P.H., STEWART, J.M. & MOCK, W.L. (1968). J.Amer.Chem.Soc. 90, 4501-4503.

BOOM, G. (1966). Accurate Lattice Parameters and the LPC Method. A Critical Investigation of the Debye—Scherrer Method. Thesis, Rijksuniversiteit te Groningen.

BUSING, W.R., MARTIN, K.O. & LEVY, H.A. (1963). ORFLS: a Fortran Crystallographic Least-Squares Program. Report ORNL-TM-305, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

BIJVOET, J.M., PEERDEMAN, A.F. & VAN BOMMEL, A.J. (1951). Nature, Lond. 168, 271-272.

BØGGILD, O.B. (1924). Kgl.Dansk.Videnskab.Selsk., Mat.fys.Medd. 6, No.3, 1-79.

GOMES DE MESQUITA, A.H. (1968). Acta Cryst. B24, 1461-1466.

International Tables for X-ray Crystallography (1968). Vol.III, 2nd ed., pp.331-338. Birmingham: Kynoch Press.

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

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

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

KARLE, I.L. & FRATINI, A.V. (1970). Acta Cryst. B26, 596-606.

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

KOJIĆ-PRODIĆ, B., ŠĆAVNIČAR, S., LIMINGA, R. & ŠLJUKIĆ, M. (1972). Acta Cryst. B28, 2028-2032.

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

LUGTENBURG, J.L. & HAVINGA, E. (1969). Tetrahedron Letters, p.2391.

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

MACHATSCHKI, F. & MUSSGNUG, F. (1942). Naturwissenschaften, 30, 106.

McWEENY, R. (1951). Acta Cryst. 4, 513-519.

NEUTRON DIFFRACTION COMMISSION, THE (1969). Acta Cryst. A25, 391-392.

PÈPE, G. & PIERROT, M. (1972). Acta Cryst. B28, 2118-2123.

ZACHARIASEN, W.H. (1945). Theory of X-ray Diffraction in Crystals. New York: John Wiley.

ÅSBRINK, S. & MAGNÉLI, A. (1959). Acta Cryst. 12, 575-581.

Fig. 1 (*cont.*)

APPENDIX III

Computing details

Recommendation 1

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

(i) A table of numerical values of F_o and F_c should always accompany a paper submitted for publication.

(ii) All parameters involved in the final calculation of structure factors should be stated.

(iii) The atomic scattering factors used should be specified precisely (including corrections for anomalous scattering if applied).

(iv) The weighting scheme adopted in least-squares calculations should be specified, (including a statement of any reflexions given zero weight).

Recommendation 2

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

(i) 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. Where appropriate, a drawing of the crystal showing the faces, their Miller indices, and the orientation of the unit-cell axes, should be supplied for deposition.

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

(iii) The correctness of the final structure should be checked, where 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.

(iv) 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).

(v) 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.

(vi) Where corrections for torsional oscillations, *etc.*, are made the molecular parameters before and after correction should be given.

Recommendation 3

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

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* *cf. International Tables for X-ray Crystallography*, Vol. III, index.

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 'New investigation of...', 'New form of...', '...from Minas Gerais' *etc.* may be added.

The *Abstract* will consist of the 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), formula, cell content, measured and calculated density, source of the material, and such other information (especially structural) as can be conveyed in approximately fifty further words.

The *Introduction* will mention 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 *thermal parameters* should be presented in a table. An indication of accuracy (preferably the standard deviation in units of the last significant figure) should be given.

Bond lengths and *bond angles* may be indicated on a Figure or (within the overall limit of length of a Short Structural Paper) in a table. If they are very numerous it may be preferable to place a table of them in a suitable depository, and mention only unusual ones (if any) in the Discussion.

The *Discussion* will contain such things as the reason for undertaking the structure determination, its chemical interest, and 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) 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 scheme (§ 10). If, for good reason, the tables are intended for publication with the paper, they should instead conform with the normal requirements (§ 5.2) 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. Acknowledgements 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.]

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, and standard deviation in the format:

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

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.*
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, and 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

The following recommendations for crystal structure papers are provided by the Committee on Chemical Crystallography of the National Academy of Sciences – National Research Council as a guide to prospective authors and their referees and editors. The purpose of this check list is to ensure that sufficient information is provided to allow critical appraisal of the results. The following format is not, nor should it be, regarded as obligatory although the information required should generally be regarded as the minimum necessary for an acceptable paper.

Manuscripts should contain each of the measured and derived quantities specified below. In every case, the estimated standard deviation, or other explicit measure of error, in these quantities should also be given. Presentation of all information should be as concise as possible.

I. *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.
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; final R value on F (if on F^2, state explicitly).
5. Brief description of overall structure, including bond lengths and angles of major interest.

II. *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 parameters; measurement temperature; radiation and wavelength; dimensions of reduced standard cell and transformation matrix to cell actually used, if different.
3. Radiation used in intensity measurement; filter(s); monochromator.
4. Z; X-ray density; measured density; method of density measurement.
5. 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*).

6. Crystal dimensions and orientation with respect to crystal axes and spindle axis; μ; absorption correction method; maximum and minimum absorption corrections.

7. Intensity measurement:
   (*a*) If film: method used to measure intensities; method of scaling intensities.
   (*b*) If diffractometer: type of geometry; detector and operating conditions: derivation of integrated intensity from measurements.
   (*c*) Measure of agreement among equivalent reflexions.
   (*d*) Method of assigning σF_{meas}: definition of unobserved reflexions.
   (*e*) Number of reflexions measured; number of independent reflexions; $(\sin\theta)/\lambda$ range within which reflexions systematically measured; total number of reflexions accessible.

III. *Structure determination and refinement*

1. Brief outline of method used: give details only if new methods are developed.
2. Computer programs; names and references.
3. Atomic scattering factors; ionization state assumed; source of scattering amplitudes.
4. Anomalous scattering. Values and sources of $\Delta f'$ and $\Delta f''$.
5. Extinction: coefficients and maximum percentage change in F_{meas}.
6. Weighting procedures:
   (*a*) Function minimized in least-squares refinement, *e.g.* $\sum w(\Delta F_{meas})^2$.*
   (*b*) Relation used between weights and estimated errors as assigned in II.7(*d*).
   (*c*) Definition of R $[\sum \Delta F_{meas}/\sum |F_{meas}|]$, S $[\sum(\Delta F_{meas}/\sigma F_{meas})^2/(m-n)]^{1/2}$,† and other indicators.
   (*d*) Treatment of unobserved reflexions; worst agreement between F_{calc} and unobserved reflexions.

IV. *Structural results*

1. Atomic coordinates; ratio of largest shift in last refinement cycle to standard deviation in coordinate given.
2. Thermal parameters (explicitly defined) and occupancy factors (if varied).
3. Interatomic distances, angles and other molecular-geometry features of major interest, including intermolecular distances; if corrections for thermal motion are made also give uncorrected values.
4. Diffraction data indicating disorder and other evidence of disorder.

V. *Structure factor tables.* Crystal-structure papers are incomplete without the evidence contained in the F_{meas}. These tables should include at least *hkl* (in some form), $|F_{meas}|$, and preferably but optionally $|F_{calc}|$. Photographic direct reproduction permits at least 2000 legible full structure factor entries per journal page.

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* $\Delta F_{meas} = ||F_{meas}| - |F_{calc}||$.
† m = number of ΔF_{meas}, n = number of variables.

Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (M. M. Woolfson, Physics Department, University of York, Heslington, York YO1 5DD, England). As far as practicable books will be reviewed in a country different from that of publication.

The Jahn–Teller effect in molecules and crystals. By R. ENGLMAN. Pp xvi+350 London: Wiley, 1972. Price £8·00.

The Jahn–Teller effect has received a great deal of attention and new understanding in the last few years. The recent progress has been made largely by new insight into the workings of the effect and the way it modifies the physical properties of systems to which it applies, namely those with degenerate or nearly-degenerate electronic states, rather than by any new mathematical formulation of the theorem itself. Much of this progress has revolved around the dynamic nature of the 'vibronic' coupling between electronic and vibrational motions, and with the introduction of new concepts the theoretical aspects of the problem have become quite complex.

This book, by a theoretician who has made a number of important contributions to several aspects of the subject, has as its objective 'to present all or most aspects of the modern Jahn–Teller effect'. This is a worthwhile aim, since most other reviews of the subject concentrate on applications to a limited class of systems, *e.g.* defects in solids, molecules, or extended systems. The author feels that there is bound to be an advantage in collecting together in one volume examples of the Jahn–Teller effect in different systems, and it is certainly interesting to be able to compare the view of the Jahn–Teller effect as seen from different vantage points. Although a variety of physical systems are included, the intention is to concentrate on the way in which the Jahn–Teller effect operates, rather than to describe in detail the physics of each system.

The degree of success in meeting these objectives varies throughout the book. In no way is this a text for the beginner attempting to get a 'feel' for the Jahn–Teller effect and an introduction to the theory. The approach throughout is to rely on references to the original work for details, and to some extent the mathematical formulation is influenced by a degree of hindsight and familiarity with the techniques involved. This is especially true in the two short introductory chapters and the long chapter 3, which presents the mathematical solutions to Jahn–Teller and pseudo-Jahn–Teller problems in localized systems (*i.e.* molecules and defects in solids). The jumping-off point for the theory is fairly advanced, and a slightly annoying feature of chapter 3 is the need to refer constantly to chapter 7 for details of the physical systems used as examples. This same problem