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 General Secretary of the International Union of Crystallography (D. W. Smits, Mathematisch Instituut, University of Groningen, Reitdiepskade 4, Groningen, The Netherlands).

International Union of Crystallography

Recommendations of the Commission on Crystallographic Computing

In crystal-structure analysis the use of the high-speed digital computer has greatly increased the amount of data which can be processed and the flexibility with which they can be interpreted. So much so that quite different opinions and standards could be maintained as to how much of these data and their interpretation should be published. The Commission on Crystallographic Computing of the Union has given consideration to this problem and has prepared some recommendations as a guide to the information that should normally be included in a publication reporting a crystal-structure analysis. The Commission has also discussed the problem of the publication of descriptions of computing methods and crystallographic computer programs, and prepared a set of recommendations in this respect.

With the approval of the Executive Committee of the Union, the recommendations have been submitted to the editors of the journals in which crystallographic papers are usually published. The full text of these statements, to which the editorial board of *Acta Crystallographica* has offered no objections, is as follows:

Recommendations on reporting the computing aspects of crystal-structure analysis

These recommendations are intended for general guidance and may not be appropriate in special cases. They are directed to ensuring a minimum quality and completeness of the reporting, and are not intended to dictate the conduct of an analysis. If adopted, they may result in a small increase in the average length of the crystal structure analysis papers, but this should be justified by the gain in precision and usefulness of the results.

We believe it is important to be able to repeat calculation, to continue refinement if necessary, and to analyze the criteria presented to establish the correctness and accuracy of the results reported.

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 the 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).

(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 reflections 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.

(ii) A final agreement index, or reliability factor (R 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 references to the author of the program in the body of the text.

Recommendations on the publication of computing methods and programs in crystallographic journals

The Commission is in favour of encouraging increased publication of material relating to crystallographic computing techniques in the journals in which crystallographers usually publish, for the following reasons:

(1) To promote a better exchange of ideas involved in computing procedures.

(2) To encourage programmers to prepare descriptions of their programs so that they can be used outside their own laboratories.

(3) To provide points of concise and exact reference for the identification of computational procedures in crystallographic papers.

(4) To provide professional recognition for programming work, which may have the same degree of scholarly and scientific merit as other material published in these journals.

Criteria Recommended for the Acceptance of Such Papers are:

1. No detailed program and no detailed descriptions written solely for a specific computer should normally be published in crystallographic journals.

2. Novel computational or programming techniques of general application in crystallography should be considered for publication as short communications or normal length papers. They should be written in general descriptive language applicable to any computer. This general description should, wherever possible, be accompanied by an algorithm or a flow diagram, which may be published with the paper (by photographic off-print) or deposited in a public depository, as deemed appropriate by the authors, referees and editors; (i.e. as for tables of F_o and F_c).

3. Descriptions of existing tested programs on particular commercial machines that are generally available to crystallographers should be considered for publication as short communications or notes. Brief descriptions such as given in the Report of the Pittsburgh Computer Conference (*Acta Cryst.* (1957), **10**, 384), are often too condensed to be useful as standard references (synoptic descriptions of this type will be provided by the *World List of Crystallographic Programs*).

The paper should contain such information as is required to make it useful as a point of reference in crystallographic papers in which the program is subsequently used. When such a brief communication is submitted for publication it should be accompanied by a separate full description such as would permit a user in another laboratory to operate the program. The paper should contain instructions for obtaining copies of this full description and of the program itself. The author should provide the referee with satisfactory evidence that the program has been adequately tested and that the description is adequate, e.g. an instance of its successful use in an independent laboratory.

4. The use of general reference languages such as ALGOL gives promise of relieving crystallographers of the recurring need to reprogram computations for new machines. Programmers should, therefore, be encouraged to make available algorithms of their computing procedures so that experience can be gained of the effectiveness with which they can be converted into machine language. In the absence of this experience, no general recommendations could be made in regard to the publication of such algorithms in crystallographic journals.

5. Papers on novel systems or devices for computing, data processing, or instrument-controlling, whether analogue or digital, should be considered for publication.

1962 Summer Schools on Crystallography

In addition to the previous notes on 1962 Summer Schools (see *Acta Cryst.* (1962), **15**, 300, ...), the I.U.Cr. Commission on Crystallographic Teaching has submitted the following information:

Brooklyn (U.S.A.): 4-15 June

Summer School on X-ray Diffraction. The lectures and laboratory work of this two-week session cover the equivalent of a six-credit lecture and laboratory graduate course. No previous X-ray experience is assumed but those with prior experience may make arrangements to undertake advanced work. At the completion of the course, registrants should be able to do most routine X-ray powder and single-crystal work.

Attendance limited to twenty-five registrants. Fee: $ 275.

Information: Mrs Doris Cattell, Special Courses, Polytechnic Institute of Brooklyn, Brooklyn 1, N.Y., U.S.A.

Gent (Belgium): 23 July–4 August

The international summer course on solid-state physics is devoted to *the optical properties of semiconductors.*

Information: Laboratorium voor Kristallografie en Studie van vaste Stoffen, Rozier 6, Gent, Belgium.

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 Theory of Crystal Structure Analysis.

By A. I. Kitaigorodskii [А. И. Китайгородский]. Translated by David and Katherine Harker. Pp. xi+275. New York: Consultants Bureau, 1961. Price $12·50.

The Russian original of this book was published in 1957. The appearance of this fluent and authoritative English translation is very welcome, and makes available to non-readers of Russian Professor Kitajgorodskij's own contributions to the problem of structure analysis, as well as his critical survey of developments originating elsewhere. In a number of places (pp. 69, 88, *etc.*) the translators have added footnotes correcting Kitajgorodskij's arguments, or expressing disagreement with his critical remarks (pp. 252, 261, *etc.*). The Russian edition has already been extensively reviewed (*Acta Cryst.* (1959), **12**, 482), and a reading of the Englich version fully confirms the great value claimed for the book by the former reviewer (who is, in fact, one of the translators). The rest of this review will, therefore, be confined to the manner of presentation rather than the matter presented.

The English edition is reproduced photographically from unjustified typescript, with the equations taken directly from the Russian original, thus excluding the possibility of new printing errors. The notation is, therefore, that familiar in continental texts: scalar product of vectors **ab**, vector product [**ab**], tg for tan, *etc.* [One usage was not familiar to the reviewer; $n!!$ is $1.3.5...n$ for n odd and $2.4.6...n$ for n even.] In general the effect of the reproduction is quite pleasant, but in some places (for example, p. 79 of the review