

19.X-1 PROPOSAL FROM THE SUBCOMMITTEE OF THE COMMISSION ON JOURNALS WITH THE CHARGE OF DEVELOPING A UNIFORM NOMENCLATURE FOR THOSE PARAMETERS THAT ARE OPERATIONALLY RELATED TO OR MEASURE THE INFLUENCE OF TEMPERATURE ON SCATTERING. By H. Hope, M.B. Hursthouse and S.E. Rasmussen.

The first recommendation of the subcommittee is to reserve the word "factor" for the full exponential expression:

$$\exp(-2\pi^2(h^2a^2U_{11}+k^2b^2U_{22}+l^2c^2U_{33}+2hka*b*U_{12}+2hla*c*U_{13}+2klb*c*U_{23}))$$

The subcommittee proposes that this expression should be called the "atomic displacement factor" when it is referred to in general terms and that it may be called "displacement factor" for short when the more complete terminology has been used previously. It is further proposed that the sequence of the U's should be: U_{11} U_{22} U_{33} U_{12} U_{13} U_{23} and that capital U implies the dimension A^2 whereas lower case u implies A. The coefficients " U_{ij} " should be called "mean square displacement coefficients" the first time they are referred to in a paper. If u_{ij} values are referred to, they should be called "rms displacement coefficients". After that, they could be called " U_{ij} coefficients" as a short notation. If authors give B_{ij} values, these could be called " B_{ij} coefficients". Other acceptable short notations could be " u_{ij} (B_{ij}) values". The use of lower case letter " b_{ij} " values for dimensionless coefficients should be discouraged.

19.X-2 STATUS OF VOLUME A. By Th. Hahn, Institut für Kristallographie der RWTH, D-5100 Aachen, Federal Republic of Germany.

The first edition of Volume A (*Space-Group Symmetry*) of *International Tables for Crystallography* appeared in November 1983 and sold out quickly. A reprint with corrections was published in the spring of 1984. The *Errata* were also published in *Acta Cryst.* (1984). A40, 485.

The second revised edition of Volume A is in press and scheduled for publication in May 1987. The main features of the revision, apart from corrections of errors, are as follows:

- Substantial modifications and amendments to several portions of text and to the list of references.
- New diagrams of improved clarity for the 17 plane groups and the 25 trigonal (including rhombohedral) space groups, prepared by R. A. Becker at Aachen. For the third edition new diagrams also for the tetragonal and hexagonal space groups are planned.
- Incorporation of two new sections on normalizers: Section 8.3.6 by H. Wondratschek, *Normalizers of Space Groups* (4 pages), deals with affine and Euclidean normalizers in the framework of space-group symmetry. Section 15 by E. Koch and W. Fischer, *Euclidean and Affine Normalizers of Space Groups and their Use in Crystallography* (14 pages), contains complete lists of the Euclidean and affine normalizers of space groups, plane groups, and point groups. Both sections provide examples, applications, and suitable references.

A *Brief Teaching Edition of Volume A* was published in June 1985. A second revised edition is in preparation.

19.X-3 STATUS OF VOLUME B. By Uri Shmueli, School of Chemistry, Tel Aviv University, Ramat Aviv, 69 978 Tel Aviv, Israel.

The purpose of the preparation of Volume B of *International Tables for Crystallography* is to present their reader/user with competent and useful accounts of the various aspects of reciprocal space in crystallographic research. The early planning of this volume was completed during the Hamburg Congress of the IUCr, and the volume was subdivided into Parts and Chapters as follows:

- Part 1. GENERAL RELATIONSHIPS AND TECHNIQUES
 - Ch. 1.1 Reciprocal Space in Crystallography [AD]
 - Ch. 1.2 The Structure Factor [AD]
 - Ch. 1.3 Fourier Methods [0]
 - Ch. 1.4 Symmetry in Reciprocal Space [AD]
- Part 2. RECIPROCAL SPACE IN CRYSTAL STRUCTURE DETERMINATION
 - Ch. 2.1 Statistical Properties of the Weighted Reciprocal Lattice [AD]
 - Ch. 2.2 Direct Methods [C]
 - Ch. 2.3 Patterson and Molecular Replacement Techniques [C]
 - Ch. 2.4 Isomorphous Replacement and Anomalous Dispersion [0]
 - Ch. 2.5 Electron Diffraction and Microscopy in Structure Determination [AD - C]
- Part 3. DUAL BASES IN CRYSTALLOGRAPHIC COMPUTING
 - Ch. 3.1 Distances, Angles and their Standard Deviations [C]
 - Ch. 3.2 Best-Plane Calculations [PD]
 - Ch. 3.3 Molecular Modelling and Graphics [AD]
 - Ch. 3.4 Accelerated Convergence of Lattice Sums [AD]
- Part 4. DIFFUSE SCATTERING AND RELATED TOPICS
 - Ch. 4.1 Thermal Diffuse Scattering of X-rays and Neutrons [C]
 - Ch. 4.2 Disorder Diffuse Scattering of X-rays and Neutrons [AD]
 - Ch. 4.3 Diffuse Scattering in Electron Diffraction [AD]
 - Ch. 4.4 Small Crystallite Size and Texture [0]
 - Ch. 4.5 Strain [0]
 - Ch. 4.6 Scattering from Mesomorphic Structures [0]
 - Ch. 4.7 Small Angle Scattering [PD]
- Part 5. DYNAMICAL THEORY AND ITS APPLICATIONS
 - Ch. 5.1 X-ray and Neutron Aspects of Dynamical Theory [0]
 - Ch. 5.2 Dynamical Theory of Electron Diffraction [AD]

The situation at the beginning of February 1987 is indicated by the symbols in square brackets: C - complete, AD - advanced draft, PD - preliminary draft, 0 - nothing in the hands of the Editor.

Various attempts have been made by the Technical Editor to establish a photocomposition procedure which accepts directly author-supplied computer-readable material. This is of particular importance when typesetting computer-generated Tables of some complexity (e.g. in Chapter 1.4).

The Editor hopes that the degree of completion of Volume B will improve by the time he reports to the Open Meeting in Perth.