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International Union of Crystallography

Acta Cryst. (1986). B**42**, 522

Commission on Journals
Author Grievance Procedure

The Commission on Journals has recently instituted a formal appeals procedure in which an author who believes his paper has been unjustifiably rejected by the Co-editor of an IUCr journal may appeal initially to the Editor of that journal for a new review and, finally, to the Editor of the other journal if the author is still aggrieved by the decision.

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Commission on Journals
Equivalent Value of the Anisotropic Temperature Factor Coefficients

Anisotropic temperature factor coefficients have been published in *Acta Cryst.* since 1979 only if the table of values is very short, or they are necessary for understanding the paper, or they possess unusual features. In all other cases, the table of values has been deposited and a brief discussion of the deposited values given instead, including the maximum and minimum values found and the presence of any nonpositive-definite coefficients determined. In addition, the equivalent values of the anisotropic temperature factors have been published, together with the list of atomic coordinates and a definition of the equivalent values in terms of the individual coefficients with source reference, see *Notes for Authors* [*Acta Cryst.* (1983), A**39**, 174-186].

Authors have been encouraged to use their definition of choice. Among the acceptable definitions are those given by W. C. Hamilton [*Acta Cryst.* (1959), **12**, 609-610] and by B. T. M. Willis & A. W. Pryor [*Thermal Vibrations in Crystallography* (1975), pp. 101-102. Cambridge Univ. Press]. Arithmetic or geometric mean values for non-orthogonal crystal axes are correct only if derived from the principal axes of the thermal ellipsoid. Values of U_{eq} are to be preferred over B_{eq}.

Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (J. H. Robertson, School of Chemistry, University of Leeds, Leeds LS2 9JT, England). As far as practicable books will be reviewed in a country different from that of publication.

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Crystallographic computing 3: Data collection, structure determination, proteins, and databases. Edited by G. M. SHELDRICK, C. KRÜGER and R. GODDARD. Pp. ix+314. Clarendon Press, Oxford, 1985. Price £25.00.

Computing methods pervade all aspects of crystallographic research and it is essential that those working in this area be aware of all recent innovations in such methods. The need is tackled in this excellent volume that represents the proceedings of the Ninth International School on Crystallographic Computing under the auspices of the IUCr Computing Commission, that was held at the Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Federal Republic of Germany, 30 July-8 August 1984, just before the International Union of Crystallography meeting in Hamburg, Germany. The international school was attended by 131 participants from 23 countries. Nine computers, ranging from a VAX 11/780 to a Rainbow personal computer, were available for use by participants at the practical sessions. There was also an Evans and Sutherland PS 300 color display unit on hand for use. Thus the stage was set for a state-of-the-art computing school, and the volume reviewed here reflects this great promise.

The range of subjects covered in this volume is divided into four sections. These consist of data collection and analysis of single crystal and powder samples, the use of data banks, program packages for maxi-, mini- and microcomputers and computing methods in protein crystallography.

The section on data collection and analysis starts with a well written article by Eric Gabe on random errors. When computing, it is essential, as Gabe points out, to avoid 'garbage in - garbage out'. It is excellent that, at the begin-

ning of the volume, we have this reminder of the importance of high-precision measurements. Crystal quality, it is stressed, should be assessed by scan methods; the care and alignment of equipment for doing this is a constant and essential task. From random errors we pass on to systematic errors and one of the most serious of these, discussed by H. D. Flack, is anomalous dispersion. Flack's discussion is timely since, with the advent of higher precision in data collection, anomalous dispersion is now being taken into account on a more routine basis than heretofore. Neglect of anomalous dispersions can (as shown, for example, by Ueki, Zalkin & Templeton in 1966) cause significant errors in atomic positions. But even if random and systematic errors are taken into account there are, as William Clegg points out, 'blunders' that can affect data. These include incorrect cell dimensions (due to 'blind reliance on automatic routines'), a poor orientation matrix, a wrongly set receiving aperture and a poor choice of standard reflections. This entire section stresses that X-ray diffraction data collection still cannot be considered a 'black box' procedure.

The chapter on the experimental determination of triplet phases and enantiomorphs is tantalizing because it is so interesting and yet not long or explanatory enough for my taste. I should have liked an expanded discussion of the use of multiple-beam X-ray diffraction to determine the phase relationship of the waves involved – I shall have to look at the references for more information. Yet the chapter must be good because it whetted my appetite with some high-precision experimental results.

Chapters then follow on computing aspects of position-sensitive detectors by Arndt and Thomas, including information on computing for the Enraf–Nonius FAST system, a chapter on a novel method of fast transmission powder diffractometry by E. R. Woelfel of the Stoe Company and an excellent chapter by Robert A. Sparks on structure refinement of powder diffraction data by the Rietveld method. Arndt and Thomas neatly categorize single-counter diffractometry as zero-dimensional data collection, moving-film photography with a layer-line screen as a two-dimensional method and screenless rotation photography as a three-dimensional method and remark that, since X-ray background in a diffraction pattern is proportional to the total volume of reciprocal space used, background must be more of a problem in the higher-dimension methods. Woelfel's chapter, involving a curved position-sensitive proportional counter with an angular range of $\Delta 2\theta = 50°$, is highly recommended. Sparks's chapter is a good overview of computer usage in powder diffractometry with explanations of the methods used.

The second section covers crystallographic data bases. G. Bergerhoff writes about the Inorganic Crystal Structure Data Base. Crystallographers have led the way in the development of data bases, with the requirements, listed by Bergerhoff, that they be complete, up to date, correct, versatile and user friendly. Some detailed examples are given. In a similar way Robin Taylor and Pella Machin each describe the use of the Cambridge Crystallographic Data File, the statistical significance of the results obtained and the use of principal-component factor analysis, in certain cases, for clarification. The needs of the user (generally a chemist) are stressed in each case. The authors pose the problem: if the chemist asks a question, is there a mechanism for answering it by use of these data bases? Errors in such usage are covered in a chapter by W. B. Schweizer.

Program systems for maxi-, mini- and microcomputers comprise the next section. Karel Huml has, happily, provided us with some invaluable lists of available crystallographic program packages. He notes the criteria for a good program package: (1) good documentation suitable for use by a novice, (2) simple input and output following IUCr and JCPDS recommendations, (3) machine independence, hence portability, (4) Fortran and (5) reliability. For powder crystallography, his lists include (with some comments) search–match program packages, indexing program packages and structure-refinement packages. For single-crystal analyses, there are annotated lists of examples of packages for Patterson methods, direct methods, structure refinement, graphics and, finally, complete single systems. What a great service and how useful to have them gathered here! Such program packages are discussed in more detail by Sid Hall who discusses portability and the use of Fortran (and Ratmac). He also reminds us about Murphy's Law that 'The more innocuous a design change appears, the further its influence will extend' (we have all experienced the problem of a small change in a computer program that has caused endless problems in unexpected places). This chapter is highly recommended. Local computers are described by Goddard, Gabe, Lee and Le Page.

George Sheldrick discusses crystallographic algorithms designed to make the most efficient use of both mini- and maxicomputer hardware and then goes on to describe *SHELX*84; this is the successor to *SHELX*76 ('written in the same inimitable style'). Henk Schenk describes higher invariants and their importance in direct methods and then goes on to introduce the direct-methods program, *SIMPEL* 83 (Schenk & Kiers). Peter Main gives a complete overview of *MULTAN*; other excellent articles include those on *DIRDIF* by Paul Beurskens (for solving the unknown part of a structure), direct methods and superstructures by R. Böhme, Patterson search methods by Christer Nordman, translation search by integrated Patterson and direct methods by Ernst Egert, and least-squares refinement and *CRYSTALS* by David Watkin. It is always nice to see an article by Peter Jones, 'Absolute structure and how not to determine it'. Finally, William Busing discusses computational models of crystals. This section is extremely interesting, explanatory and informative. Each chapter is first rate.

The final section is on computer methods in protein crystallography. Wayne Hendrickson discusses anomalous dispersion. He describes the uses of anomalous scattering to determine absolute configuration, to locate native metal centers in proteins (as he did for crambin) and to supplement isomorphous replacement phasing. Jones and Pflugrath describe the use of the computer graphics program *FRODO* for electron density map fitting. The volume contains many practical instructions that will be useful to the new user; *FRODO* can use coordinates or an electron density map or a vector data set. A. G. W. Leslie describes combined constrained/restrained refinement (*CORELS*) and the ways in which the problem of maintaining good stereochemistry at the junction of constrained groups is handled by this program; the application to a protein, of four identical subunits each with a molecular weight of 36 000, is described in detail. *CORELS* can be used to study conformational changes on ligand binding and to eliminate errors in a structural model before going on

to use a restrained-least-squares refinement program. Restrained least-squares refinement for proteins is discussed by Wayne Hendrickson. As proteins are so large some way of reducing the number of entries in the normal matrix is needed.

This book is highly recommended for every laboratory (and computer room) bookshelf. It contains the old and the new, the practical and the thoughtful, and covers a wide range of topics with many good references. I raise one adverse criticism on the production of this photo-offset book; namely, the quality of printing of some of the articles. Certain chapters, produced faintly by a dot-matrix printer, are very difficult to read. They would have been better if they had been retyped or type-set. Apart from this the editors have done a first-class job of producing an up-to-date volume covering advances in computing in crystallography.

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Structural chemistry of silicates: structure, bonding, and classification. By F. LIEBAU. Pp. xiii+347, 136 figures. Berlin, Heidelberg, New York, Tokyo: Springer-Verlag, 1985. Price DM 163.00.

'The hardness of men's hearts makes an idol of classification, *but a knowing heart will use it as an aid*'. Thus ends this remarkable book with an optimistic twist by the author (in italics) of a statement by Samuel Butler. Silicates are perhaps among the least lauded of substances in human societies. Yet, six silicate species comprise about 95 volume % of the Earth's crust. They play an essential economic role from stained-glass windows and wine goblets to building stone, from computer chips to bricks and concrete. Without silicates and their products, civilization as we know it would not exist.

A very readable and highly informative book, it can be easily incorporated into a graduate level course sequence, particularly in ceramics, structural inorganic chemistry and the earth sciences. A bibliography with over 650 references to nearly every significant publication on silicate crystal chemistry is a valuable aid for literature search. The figures – most of them displaying scaled crystal structures – are elegantly crafted. A most important feature, rarely noted in such treatises, is the complementary and uniform quality of these drawings.

Ten major chapters comprise the book. Aspects of chemical crystallography make up six (Chapters 4, 5, 6, 7, 9 and 10). Chapter 4 is of key importance, for it reveals the symbols and principles behind silicate anion nomenclature. Because $[^{[4]}Si^{4+}O_4]^{4-}$ has mesodesmic properties, silicates polymerize in bewildering variety and to this day, a rationalization of rules for predicted silicate polymerization does not exist. Important classificatory principles involve the connections of the silicate polyhedra, usually tetrahedra. Linkedness (L) involves topologic fusions of the polyhedra (corners, edges, faces), connectedness (S) refers to the available corner-sharing elements, and branchedness (B) refers to the secondary dendrites which attach to the central spine and five types are discerned. The dimensionality (D) refers to the space in which the Si_xO_y cluster is described and multiplicity (M) to further polymerizations of similar units within the same space to form a larger aggregate in that space. Finally, a diversity of chain lengths in SiO_4 units can exist, the periodicity (P). The German word for the number of polyhedra before a chain segment translationally repeats followed by -er, specifies the periodicity. Alamosite, $Pb_{12}[Si_{12}O_{36}]$, is one of the largest, a *zwölfer* chain.

The remarkable feature of this book is its thoroughness. The description and portrayal of crystal structures is wonderfully reviewed in Chapter 2. Very few textbooks on mineral structure (and there are many!) do justice to this problem. Chemical bonding theory in all its ramifications appears in Chapter 3. Chapter 8 reviews the other classifications of silicates. This is another rich lode. Yet it is clear no classification is absolute. A classification must always serve some purpose (an added bonus would be built-in predictability of general properties, but this is rare!). This one, I believe, is an efficient working classification, a means toward sensible taxonomy and information retrieval. It is a language of crystal structure. Unfortunately, not all bases can possibly be covered. For example, I would create a new radical class for all $2r[Si_{2p}O_{5p}]$ (r = ring, p = number of tetrahedra in a ring), the so-called double rings. All these map with their connectivities conserved on a sphere. Recently, I was involved with the giant $[Si_{48}O_{120}]$ core in ashcroftine, but $p \neq 24$! It defines the truncated cuboctahedron, an Archimedean semiregular solid. All of these silicates whose connectivities define maps on a sphere, define polyhedra.

A magnificent book! At least ten years of effort went into it. The uniformity of figures, the sensibility of the tables, the beautiful layout, the thorough coverage and above all a book which befriends the reader (freely translating a remarkable late Bach cantata '... And take me by your hand/and gently lead me on.'). I doff my hat to author and publisher.

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Diamond. By G. DAVIES. Pp. x+255. Bristol: Adam Hilger, 1984. Price £17.50, US $28.00.

This is a delightful book, written not for the diamond specialist, but for the intelligent layman. Focusing on a single topic such as diamond might seem to be very narrow, even if glamorous, but the author leads the reader through wide-ranging tracts of solid state physics, surface physics, spectroscopy, chemistry and geology, not to mention history, politics, economics and gemology, whose variety and interest are an intellectual feast, educative and entertaining in the best sense.