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## **International Union of Crystallography**

Acta Crvst. (1986). B42, 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.

Acta Cryst. (1986). B42, 522

## **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 STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). J. Chem. Phys. 42, 3175-3187.

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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), A39, 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 nonorthogonal crystal axes are correct only if derived from the principal axes of the thermal ellipsoid. Values of  $U_{e0}$  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 LS29JT, England). As far as practicable books will be reviewed in a country different from that of publication.

Acta Cryst. (1986). B42, 522-524

Crystallographic computing 3: Data collection, structure determination, proteins, and databases. Edited by G. M. SHELDRICK, C. KRÜGER and R. GOD-DARD. 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-