The authors would like to thank Professor B. E. Robertson, University of Regina, Regina, Canada, for pointing out the typographical error in the c axis of this structure.

Reference


The structure of gentiobiose: erratum. By D. C. ROHRER, Medical Foundation of Buffalo, Inc., Buffalo, NY 14203, USA, and A. SARKO, T. L. BLUHM and Y. N. LEE, Department of Chemistry, State University of New York, College of Environmental Science and Forestry, Syracuse, NY 13210, USA

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Abstract

A typesetting error is corrected. In the paper by Rohrer, Sarko, Bluhm & Lee [Acta Cryst. (1980), B36, 650–654] the y coordinate for atom O(6') in Table 1 is incorrect. The correct value is 16057 (5).

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Book Review

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.


Nowadays the majority of crystal structures are solved by means of a black box, called: 'direct methods computer program'. Professional knowledge is required to bypass program pitfalls, and to solve 'troublesome' cases which, although relatively few in number, often require a great deal of computing time, as well as human time and invention. Therefore, many expert crystallographers are still working on the improvement of the methods.

In 1980 two new books on direct methods were welcomed: Theory and Practice of Direct Methods in Crystallography has been reviewed [Acta Cryst. (1980), B36, 2860]; here we praise Direct Methods in Crystallography by Carmelo Giacovazzo: an excellent book covering a wealth of mathematical—statistical techniques, formulae, methods, and literature references. We agree with the author that 'Specialists will find good coverage of existing results in addition to various new pieces of material. A serious attempt has been made to amalgamate into a logical order a vast variety of scientific contributions with all their differing approaches. Almost all theoretical contributions are believed to have been reviewed in compiling this volume.'

Chapters 1 and 2 cover Wilson statistics, statistical effects of space-group symmetry, the symmetry enhancement factor (Wilson's p, and Karle and Hauptman's e), absolute scaling of the intensities, normalization, the origin problem, invariants and semi-invariants ('seminvariants'), and enantiomorph definition (56 + 49 pages).

Chapter 3 (The Algebraic Relationships between Structure Factors) is an important chapter which very concisely treats the Sayre equation, the Σ2 relationship, the quartet relationship, the B3,0 formula (eq. 3.57) and many related topics (37 pages).

Chapters 4 and 5 list inequalities among structure factors (including the Karle–Hauptman determinant) and Σ1 relationships (26 + 14 pages).

Chapter 6 gives a description of the Sayre–Hughes and tangent methods. It includes sections entitled 'From partial to complete structure' and 'Figures of merit'. This chapter is much too short to be a practical guide, yet it beautifully summarizes the contents of the various black boxes! (49 pages).

Chapters 7 and 8 give a thorough treatment of the underlying theory (joint probability distributions; Giacovazzo's representation theory) which, for instance, leads to the estimation of phases for quartets and seminvariants (45 + 100 pages).

Some useful appendices offer students an account of the mathematics involved (37 pages).
This work will be of great value not only for direct-methods experts, but also for crystallographers who are involved in the study of methods where the statistical properties of structure factors play a role. It will earn its place in every crystallographic library. Because of its extensive treatment of the mathematical aspects of direct methods, and the lesser emphasis on the practical applications, the book is less suitable for students beginning direct methods.

Finally, the publishers have done a good job on the presentation of the book.

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**Acta Cryst.** (1981). **B37**, 1802

**Book Received**

The following book has been received by the Editor. Brief and generally uncritical notices are given of works of marginal crystallographic interest; occasionally a book of fundamental interest is included under this heading because of difficulty in finding a suitable reviewer without great delay.