References

CRESENZI, V., CESARO, A. & RUSSO, E. (1973). Int. J. Peptide Protein Res. 5, 427–434.

DEGEILH, R. & MARSH, R. E. (1959). Acta Cryst. 12, 1007–1014.

FURNAS, T. C. JR & HARKER, D. (1955). Rev. Sci. Instrum. 26, 449–453.

GERMAIN, G., MAIN, P. & WOOLFSON, M. M. (1971). Acta Cryst. A27, 368–376.

IUPAC–IUB COMMISSION ON BIOCHEMICAL NOMENCLATURE (1970). J. Mol. Biol. 52, 1–17.

NAHRINGBAUER, I. (1978). Acta Cryst. B34, 315–318.

SHORT COMMUNICATIONS

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.

Structure of diacetylmorphine (heroin): erratum. By DENNIS V. CANFIELD, *Forensic Science Coordinator, University of Southern Mississippi, Hattiesburg, MS 39401, USA*

Abstract

A typographical error in the *c* axis of diacetylmorphine |Canfield, Barrick & Giessen (1979), *Acta Cryst.* B35, 2806–2809| is corrected and the new torsion angles, bond lengths, and bond angles are reported. The correct value for the *c* axis is 16·092 (7) Å.

The *c* axis in diacetylmorphine was previously reported (Canfield, Barrick & Giessen, 1979) as 16·392 (7) Å, when in fact it should be 16·092 (7) Å. This typographical error
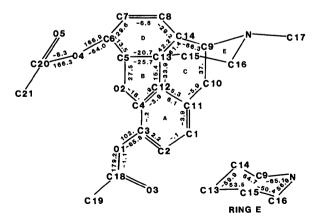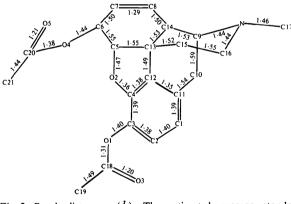

Fig. 2. Bond distances (Å). The estimated average standard deviation in the bond lengths is 0·014 Å.

occurred after the structure was determined. However, the incorrect value was used to calculate the torsion angles and bond lengths reported. The correct bond lengths and torsion angles are given in Figs. 1 and 2. The contact distances O(5)–C(19) and O(3)–C(21) reported in the original paper should be 3·222 (25) and 3·289 (20) Å respectively. Corrected bond angles have been deposited.*

---

* A list of corrected bond angles has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36164 (2 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Fig. 1. Configurational drawing of diacetylmorphine with endocyclic torsion angles (°) for rings *A*, *B*, *C*, *D*, and *E*. The estimated average standard deviation in the torsion angles is 1·5°.

Reference

CANFIELD, D., BARRICK, J. & GIESSEN, B. C. (1979). *Acta Cryst.* B**35**, 2806–2809.

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*

Abstract

A typesetting error is corrected. In the paper by Rohrer, Sarko, Bluhm & Lee [*Acta Cryst.* (1980), B**36**, 650–654] the *y* coordinate for atom O(6′) in Table 1 is incorrect. The correct value is 16057 (5).

All relevant information is given in the *Abstract*.

Book Review

Direct methods in crystallography. By CARMELO GIACOVAZZO. Pp. xv + 432. London and New York: Academic Press, 1980. Price £37·80, US $87.00.

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), B**36**, 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 ε), 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 Σ_2 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 Σ_1 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).