



Fig. 4. Stramonin-B (left), bromohelenalin (middle), and the superposition of the two pseudoguaianolides (right). The atoms superimposed are those of the bicyclic ring system C(1) through C(10) [see (1)] by minimizing $\sum d_i^2$, the sum of the squares of the distances between corresponding atomic positions in the two molecules (see text).

half chair. The average torsion-angle magnitude in the ring is 57.9° . A pseudo diad axis relates ring atoms on either side of the line from C(10) to the midpoint of the C(6)–C(7) bond. The C(15) methyl group is antiperiplanar to C(8).

The pseudoguaianolides are subdivided into two main families. Stramonin-B belongs to the Ambrosia class in which the lactone is *cis*-attached to C(6) and C(7). The other class is the Helenium family in which the lactone is *cis*-attached to C(7) and C(8). In addition to differing modes of lactone bonding, the Ambrosia and Helenium classes differ in their stereochemistry at C(10). Bromohelenalin (Mazhar-ul-Haque & Caughlan, 1969) is a representative of the Helenium class and has been compared to the observed structure of stramonin-B, Fig. 4. In spite of their differing stereochemistries, the two pseudoguaianolides have remark-

ably similar conformations. Using a routine similar to one described by Nyburg (1974) which has been used successfully in the comparative analysis of molecular conformation, the structures of stramonin-B and bromohelenalin were fitted together by a least-squares method. Atomic positions fitted in the two molecules were atoms C(1) through C(10). The average separation between corresponding atoms is only 0.06 Å and the maximum separation is 0.1 Å between the atoms C(10) and C(3) in corresponding molecules.

This work was supported in part by PSH Grants AM19856 and CA13689. We thank Douglas Rohrer for making the least-squares fitting routine *FITMOL* available to us and for supervising the data collection.

References

- CROMER, D. T. & WABER, J. T. (1974). *International Tables for X-ray Crystallography*, Vol. IV, p. 71. Birmingham: Kynoch Press.
- DUAX, W. L., WEEKS, C. M. & ROHRER, D. C. (1976). *Stereochemistry*, Vol. 9, edited by N. L. ALLINGER & E. L. ELIEL. New York: John Wiley.
- GRIECO, P. A., OGURI, T., BURKE, S., RODRIQUEZ, E., DETITTA, G. T. & FORTIER, S. (1978). *J. Org. Chem.* **43**, 4552–4554.
- LANGS, D. A. & DETITTA, G. T. (1975). *Acta Cryst.* **A31**, S16.
- MAZHAR-UL-HAQUE & CAUGHLAN, C. (1969). *J. Chem. Soc. B*, pp. 956–960.
- NYBURG, S. (1974). *Acta Cryst.* **B33**, 816–824.
- RODRIQUEZ, E. (1977). *Biochem. Syst. Ecol.* **5**, 207–218.
- STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). *J. Chem. Phys.* **42**, 3175–3187.
- STOUT, G. H. & JENSEN, L. H. (1968). *X-ray Structure Determination. A Practical Guide*, p. 457. London: Macmillan.

SHORT COMMUNICATIONS

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Acta Cryst. (1979). **B35**, 1744

Equatorial 2-phenoxy-*trans*-1-oxadecalin: erratum. By PETER G. JONES, OLGA KENNARD, SOSALE CHANDRASEKHAR and ANTHONY J. KIRBY, *University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, England*

(Received 13 March 1979; accepted 19 March 1979)

Abstract

An error in the paper by Jones, Kennard, Chandrasekhar & Kirby [*Acta Cryst.* (1978). **B34**, 3835–3837] is corrected.

omitted. Line 4 of page 3836 should read as follows: Gorenstein & Kar (1977). Similarly the angle O(1)–C(2)–C(3) is 111.5° in (I), compared with 113.1° in the axial isomer. This angle must open to...

Reference

- JONES, P. G., KENNARD, O., CHANDRASEKHAR, S. & KIRBY, A. J. (1978). *Acta Cryst.* **B34**, 3835–3837.

The third sentence of the *Discussion* of a previous paper (Jones, Kennard, Chandrasekhar & Kirby, 1978) was

0567-7408/79/071744-01\$01.00

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