Although the specific relevance of these structural differences is not understood fully at present, it seems logical to expect the substituents on C(2), C(3) and C(5) to influence the minimum-energy (preferred) orientations of the 4-phenyl and 4-OCOEt relative to the piperidine ring. As well as spatial requirements for the C(4) substituents, the vital factor for analgesic activity remains the accessibility of the lone pair on the N atom for interaction with the receptor as suggested by Belleau, Conway, Ahmed & Hardy (1974) and supported by comparison of the crystal structures of two isomers of the rigid 16,17-butanomorphinan-3-ol (Ahmed, 1981). The stereoelectronic nature of this interaction was discussed by Dimaio, Ahmed, Schiller & Belleau (1979).

The solid-state conformations of the isomers for (I), (II) and (III) are characterized by a piperidine ring in the chair form and an equatorial phenyl, except for the two crystalline forms of β-promedol alcohol, whose ester is the most active isomer of (II). There, the phenyl ring adopts an axial position while the piperidine ring remains in the chair form. The main features of an axial phenyl configuration are (1) the OH and the lone pair of the N atom are *cis*, (2) the phenyl ring has very little freedom of re-orientation through a twist about C(4)–C(10) (obvious from Fisher–Hirschfelder–Taylor atom model), and (3) the N···O separation is increased from 3·42–3·58 Å to 4·16–4·20 Å when the phenyl is equatorial. Further systematic comparisons with other analgesics are needed to ascertain which of the two conformations is the one actually adopted during interaction with the receptor.

The authors thank Dr A. F. Casy of the School of Pharmacy, University of Bath, for supplying the crystals and commenting on the discussion, and Mrs M. E. Pippy for assistance with the computations.

References

AHMED, F. R. (1981). *Acta Cryst.* B37, 188–192.

AHMED, F. R. & BARNES, W. H. (1963). *Acta Cryst.* **16**, 1249–1252.

AHMED, F. R. & DE CAMP, W. H. (1972). *Acta Cryst.* B28, 3489–3494.

AHMED, F. R., HALL, S. R., PIPPY, M. E. & HUBER, C. P. (1973). The *NRC* System of Crystallographic Computer Programs for the IBM/360. Accession Nos. 133–147 in *J. Appl. Cryst.* **6**, 309–346.

BELLEAU, B., CONWAY, T., AHMED, F. R. & HARDY, A. D. (1974). *J. Med. Chem.* **17**, 907–908.

CASY, A. F. (1978). *Prog. Drug Res.* **22**, 149–227.

CASY, A. F. (1982). *Med. Res. Rev.* **2**, 167–192.

CASY, A. F., OGUNGBAMILA, F. O. & ROSTRON, C. (1982). *J. Chem. Soc. Perkin Trans.* 1, pp. 749–753.

CYGLER, M., AHMED, F. R., CASY, A. F. & OGUNGBAMILA, F. O. (1981). *Acta Cryst.* A37, C-59.

DE CAMP, W. H. & AHMED, F. R. (1972*a*). *Acta Cryst.* B28, 1791–1796.

DE CAMP, W. H. & AHMED, F. R. (1972*b*). *Acta Cryst.* B28, 1796–1800.

DE CAMP, W. H. & AHMED, F. R. (1972*c*). *Acta Cryst.* B28, 3484–3489.

DIMAIO, J., AHMED, F. R., SCHILLER, P. & BELLEAU, B. (1979). *Recent Advances in Receptor Chemistry*, edited by F. GUALTIERI, M. GIANNELLA & C. MELCHIORRE. Amsterdam: Elsevier/North-Holland Biomedical Press.

HANSON, H. P., HERMAN, F., LEA, J. D. & SKILLMAN, S. (1964). *Acta Cryst.* **17**, 1040–1044.

JACOBSON, A. E. (1980). Private communication.

JOHNSON, C. K. (1971). *ORTEP*II. Report ORNL-3794, 2nd revision. Oak Ridge National Laboratory, Tennessee.

KARTHA, G., AHMED, F. R. & BARNES, W. H. (1960). *Acta Cryst.* **13**, 525–531.

MAIN, P., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1978). *MULTAN*78. *A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.

MISTRYUKOV, E. A. & SHVETSOV, N. I. (1961). *Bull. Acad. Sci. USSR, Div. Chem. Sci.* pp. 268–269.

PORTOGHESE, P. S. (1978). *Acc. Chem. Res.* **11**, 21–29.

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

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.

Acta Cryst. B40, 440

Books Received

The following books have 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.

Vectors and tensors in crystallography. By DONALD E. SANDS. Pp. xvi+228. Reading, MA: Addison-Wesley Advanced Book Program/World Science Division, 1982. Price US $26.50. A review of this book, by J. Kopf, has been published in the May issue of *Acta Crystallographica*, Section A, p. 312.

The structure of non-crystalline materials, 1982. Edited by P. H. GASKELL, J. M. PARKER & E. A. DAVIS. Pp. xiii+609. London: Taylor & Francis, 1983. Price £28.00, US $62.00. A review of this book, by J. H. Robertson, has been published in the July issue of *Acta Crystallographica*, Section A, p. 488.

Fourier optics: an introduction. By E. G. STEWARD. Pp. 185. Chichester: Ellis Horwood Ltd (John Wiley & Sons), 1983. Price £15.00 (hard cover), £7.95, US $13.75 (paper). A review of this book, by A. D. Booth, has been published in the July issue of *Acta Crystallographica*, Section A, p. 487.