1984). For the preparation see Nagano, Mori, Takaku, Matsunaga, Kujirai, Ogasawara, Sugano & Shindoh (1984).

References

FRENZ, B. A. (1984). *Structure Determination Package*. College Station, Texas, USA, and Enraf–Nonius, Delft, The Netherlands.

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)

JOHNSON, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

MAIN, P., FISKE, S. J., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1982). *MULTAN*11/82. *A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data*. Univs. of York, England, and Louvain, Belgium.

NAGANO, H., MORI, T., TAKAKU, S., MATSUNAGA, I., KUJIRAI, T., OGASAWARA, T., SUGANO, S. & SHINDOH, M. (1984). Japanese Patent 1,186,252.

SAKAI, K., AKIMA, M., HINOHARA, Y. & OBATAKE, N. (1984). *J. Pharm. Pharmacol.* **36**, 175–181.

Acta Cryst. (1987). C**43**, 2462–2463

Structure of Propionanilide Derivative AN132

BY YOSHIHARU NAWATA,* YASUYUKI KATOH, MICHIO TAKAGI AND KIYOSHIGE OCHI

Research Laboratories, Chugai Pharmaceutical Co. Ltd, Takada, Toshima, Tokyo 171, *Japan*

(*Received* 1 *June* 1987; *accepted* 15 *July* 1987)

Abstract. 3-{*N*-[2''-(*N'*,*N'*-Diisopropylamino)]ethylamino}-2',6'-dimethylpropionanilide (AN132), $C_{19}H_{33}NO_3$, $M_r = 319{\cdot}49$, orthorhombic, *Pbca*, $a = 21{\cdot}628\ (2)$, $b = 22{\cdot}542\ (2)$, $c = 8{\cdot}326\ (1)$ Å, $V = 4059{\cdot}2$ Å^3, $Z = 8$, $D_x = 1{\cdot}046$ g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 4{\cdot}75$ cm^{-1}, $F(000) = 1408$, $T = 298$ K, final $R = 0{\cdot}054$ for 1155 unique reflections [$F_o^2 > 2\sigma(F_o^2)$]. The amide group, connecting a benzene ring and a zigzag chain, is approximately perpendicular to both best planes. The carbonyl O atom forms intermolecular H bonds with two –NH groups in an adjacent molecule.

Experimental. Colorless needles of AN132 grew from isopropyl ether. Crystal size 0·43 × 0·13 × 0·05 mm, Enraf–Nonius CAD-4 κ-cradle diffractometer, Cu $K\alpha$ radiation, graphite monochromator, θ–2θ scan with scan speed 2·75–4·12° min^{-1} in θ, scan width (0·55 + 0·14tanθ)°. Range of indices $0 \le h \le 26$, $0 \le k \le 27$, $0 \le l \le 10$ ($2\theta < 140°$). Lattice constants determined based on 25 2θ values ($16 < 2\theta < 49°$). Variation of standard < 4·1%; 3839 unique reflections measured; 1155 observed reflections with $F_o^2 > 2\sigma(F_o^2)$. Systematic absences 0*kl*, *k* odd; *h*0*l*, *l* odd; *hk*0, *h* odd. No corrections for absorption. Structure solved by direct methods with *MULTAN*11/82 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982). Refined by full-matrix least squares. The locations of H atoms were calculated stereochemically, except for that of H(11) found from difference Fourier map. Non-H atoms refined with anisotropic thermal parameters, and H atoms with isotropic thermal parameters (B = 5·0 Å^2: fixed). $\sum w(|F_o| - |F_c|)^2$ minimized; $w = 1{\cdot}0$ for $F_o < 472{\cdot}6$, $w = (472{\cdot}6/F_o)^2$ for $F_o \ge 472{\cdot}6$. Final $R = 0{\cdot}054$, $wR = 0{\cdot}047$, $S = 3{\cdot}90$ for 341 variables, secondary-extinction factor (g) 1·3 (1) × 10^{-7} [$|F_o| = |F_c|/(1+gI_c)$]; $\Delta/\sigma < 1{\cdot}1$, largest peak in final ΔF map +0·16 e Å^{-3}; atomic scattering factors from *International Tables for X-ray Crystallography* (1974); programs: Enraf–Nonius *SDP* (Frenz, 1984), *ORTEP*II (Johnson, 1976). The structure of AN132 is shown in Fig. 1; a projection of the crystal structure is shown in Fig. 2. Positional parameters and equivalent values of the anisotropic temperature factors are given

Table 1. *Final fractional coordinates and equivalent isotropic temperature factors for non*-H *atoms with e.s.d.'s in parentheses*

$B_{eq} = \frac{4}{3}\sum_i\sum_j B_{ij}\mathbf{a}_i\mathbf{a}_j$.

	x	y	z	B_{eq}(Å^2)
C(1)	0·4098 (2)	0·2546 (3)	0·3756 (7)	4·6 (1)
C(2)	0·4506 (3)	0·2117 (3)	0·4271 (8)	6·4 (2)
C(3)	0·5044 (3)	0·2297 (4)	0·505 (1)	9·5 (2)
C(4)	0·5160 (3)	0·2882 (4)	0·5292 (9)	10·0 (3)
C(5)	0·4766 (3)	0·3296 (3)	0·4778 (8)	7·7 (2)
C(6)	0·4217 (3)	0·3129 (3)	0·4021 (6)	5·3 (2)
N(7)	0·3558 (2)	0·2369 (2)	0·2931 (5)	4·9 (1)
C(8)	0·3080 (3)	0·2095 (2)	0·3615 (7)	4·4 (1)
C(9)	0·2534 (3)	0·1959 (2)	0·2553 (7)	5·3 (1)
C(10)	0·1988 (3)	0·2320 (3)	0·3034 (7)	5·4 (2)
N(11)	0·2135 (2)	0·2942 (2)	0·3032 (5)	5·1 (1)
C(12)	0·1610 (3)	0·3327 (3)	0·3345 (7)	5·6 (2)
C(13)	0·1806 (3)	0·3969 (3)	0·3355 (8)	6·2 (2)
N(14)	0·1290 (2)	0·4361 (2)	0·3687 (6)	5·5 (1)
C(15)	0·0925 (3)	0·4509 (3)	0·2314 (9)	8·4 (2)
C(16)	0·1133 (5)	0·4908 (7)	0·114 (1)	20·7 (5)
C(17)	0·1404 (3)	0·4835 (3)	0·4797 (9)	8·4 (2)
C(18)	0·1414 (6)	0·4612 (4)	0·640 (1)	16·7 (4)
C(19)	0·1991 (4)	0·5185 (4)	0·457 (2)	17·3 (4)
C(20)	0·4417 (3)	0·1480 (3)	0·397 (1)	9·7 (2)
C(21)	0·3762 (3)	0·3596 (3)	0·3514 (8)	7·3 (2)
O(22)	0·3078 (2)	0·1965 (2)	0·5051 (4)	5·32 (9)
C(23)	0·0265 (4)	0·4675 (3)	0·275 (1)	9·8 (2)

* To whom all correspondence should be addressed.

0108-2701/87/122462-02$01.50

in Table 1; bond distances and angles are listed in Table 2.*

Related literature. The title compound has antiarrhythmic activity. For the preparation and medicinal action see Takagi, Yamazaki & Katoh (1987).

* Lists of anisotropic thermal parameters, structure factors, torsion angles, least-squares planes and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44256 (24 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

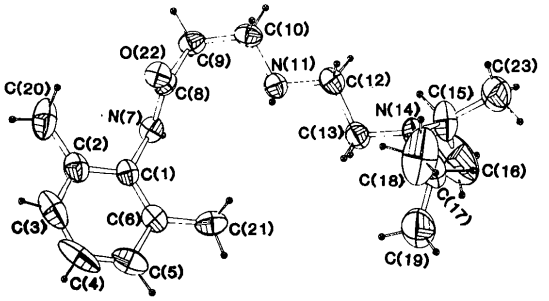

Fig. 1. A perspective view of the molecule with the numbering scheme.

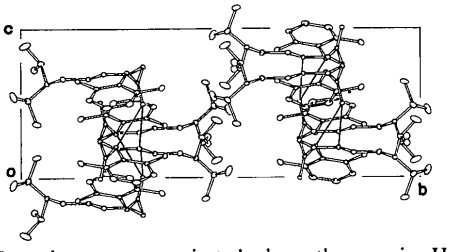

Fig. 2. Crystal structure projected along the *a* axis. Hydrogen bonds are indicated by single lines.

Table 2. *Bond lengths* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

C(1)–C(2)	1·377 (8)	C(9)–C(10)	1·489 (8)
C(1)–C(6)	1·357 (9)	C(10)–N(11)	1·438 (7)
C(1)–N(7)	1·413 (7)	N(11)–C(12)	1·453 (7)
C(2)–C(3)	1·391 (9)	C(12)–C(13)	1·507 (9)
C(2)–C(20)	1·470 (10)	C(13)–N(14)	1·451 (8)
C(3)–C(4)	1·357 (12)	N(14)–C(15)	1·429 (9)
C(4)–C(5)	1·334 (11)	N(14)–C(17)	1·434 (9)
C(5)–C(6)	1·396 (9)	C(15)–C(16)	1·404 (15)
C(6)–C(21)	1·502 (9)	C(15)–C(23)	1·519 (11)
N(7)–C(8)	1·332 (7)	C(17)–C(18)	1·428 (12)
C(8)–C(9)	1·507 (8)	C(17)–C(19)	1·508 (11)
C(8)–O(22)	1·231 (6)		

C(2)–C(1)–C(6)	120·5 (5)	C(9)–C(8)–O(22)	121·3 (5)
C(2)–C(1)–N(7)	118·9 (5)	C(8)–C(9)–C(10)	110·7 (5)
C(6)–C(1)–N(7)	120·6 (5)	C(9)–C(10)–N(11)	110·8 (5)
C(1)–C(2)–C(3)	118·4 (6)	C(10)–N(11)–C(12)	114·1 (4)
C(1)–C(2)–C(20)	123·3 (6)	N(11)–C(12)–C(13)	110·8 (5)
C(3)–C(2)–C(20)	118·3 (6)	C(12)–C(13)–N(14)	111·7 (5)
C(2)–C(3)–C(4)	120·6 (7)	C(13)–N(14)–C(15)	114·6 (5)
C(3)–C(4)–C(5)	120·9 (7)	C(13)–N(14)–C(17)	116·4 (5)
C(4)–C(5)–C(6)	119·9 (7)	C(15)–N(14)–C(17)	115·9 (5)
C(1)–C(6)–C(5)	119·8 (6)	N(14)–C(15)–C(16)	122·1 (7)
C(1)–C(6)–C(21)	120·6 (5)	N(14)–C(15)–C(23)	112·8 (6)
C(5)–C(6)–C(21)	119·6 (6)	C(16)–C(15)–C(23)	108·0 (7)
C(1)–N(7)–C(8)	124·4 (5)	N(14)–C(17)–C(18)	110·0 (7)
N(7)–C(8)–C(9)	116·8 (5)	N(14)–C(17)–C(19)	116·9 (7)
N(7)–C(8)–O(22)	121·9 (5)	C(18)–C(17)–C(19)	107·0 (8)

References

FRENZ, B. A. (1984). *Structure Determination Package.* College Station, Texas, USA, and Enraf–Nonius, Delft, The Netherlands.

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)

JOHNSON, C. K. (1976). *ORTEPII.* Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

MAIN, P., FISKE, S. J., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1982). *MULTAN11/82. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.

TAKAGI, M., YAMAZAKI, T. & KATOH, T. (1987). *Kokai Tokkyo Koho* (Japanese Patent), No. 62-30746.

Acta Cryst. (1987). C**43**, 2463–2465

7,7-Dichloro-4-(diphenylmethylene)bicyclo[3.2.0]hept-2-en-6-one

BY WILLIAM H. WATSON* AND ANTE NAGL†

Department of Chemistry, Texas Christian University, Fort Worth, Texas 76129, *USA*

(*Received* 6 *July* 1987; *accepted* 14 *July* 1987)

Abstract. $C_{20}H_{14}Cl_2O$, $M_r = 341{\cdot}24$, monoclinic, $P2_1/a$, $a = 9{\cdot}324$ (1), $b = 18{\cdot}704$ (3), $c = 9{\cdot}754$ (1) Å, $\beta = 107{\cdot}06$ (1)°, $V = 1626{\cdot}3$ (4) Å^3, $Z = 4$, $D_x = 1{\cdot}39$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 3{\cdot}99$ cm^{-1}, $F(000) = 704$, $T = 293$ K, $R = 0{\cdot}0552$ for 1718 independent observed reflections. The five-membered ring is in an envelope conformation with C(5) the flap. The four-membered ring is folded by 15·9 (6)° along C(1)···C(6). The planes of the two phenyl rings are twisted by 78·4 (7)° and form interplanar angles of

* Author to whom correspondence should be addressed.

† On leave from Faculty of Technology, University of Zagreb, Zagreb, Yugoslavia.

0108-2701/87/122463-03$01.50