squares structural parameters are given in Table 1.* Bond distances and bond angles are listed in Table 2.

The acetyl substituent is in the 7β position of the 6,14-ethenomorphinan skeleton, and differs from the position observed in the Diels–Alder addition product of 6-demethoxythebaine (van Koningsveld, Maat & Lie, 1984). Obviously, opening of the 4,5-epoxy ring in 6-demethoxythebaine results in cycloaddition from the other side of the diene system. Consequently, the reaction products of the title compound with *e.g.* different Grignard compounds will possess a structure with the alkyl methyl carbinol substituent also in the 7β position. These structures are based on morphinans with a rigid structure and less oxygen-containing substituents than morphine itself.

A novel class of potentially interesting 7β-substituted 6,14-ethenomorphinans becomes herewith accessible for the study of structure–activity relationships of analgesics.

* Lists of structure factors, anisotropic temperature factors, H-atom parameters and distances and angles involving H atoms have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39637 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

CRABBENDAM, P. R., LIE, T. S., LINDERS, J. T. M. & MAAT, L. (1984). To be published.

GERMAIN, G., MAIN, P. & WOOLFSON, M. M. (1971). *Acta Cryst.* A**27**, 368–376.

JOHNSON, C. K. (1965). *ORTEP*. Report ORNL-3794, revised June 1970. Oak Ridge National Laboratory, Tennessee.

KONINGSVELD, H. VAN , LIE, T. S. & MAAT, L. (1984). *Acta Cryst.* C**40**, 313–314.

KONINGSVELD, H. VAN, MAAT, L. & LIE, T. S. (1984). *Acta Cryst.* C**40**, 1082–1084.

STEWART, J. M., KRUGER, G. J., AMMON, H. L., DICKINSON, C. W. & HALL, S. R. (1972). The *XRAY*72 system – version of June 1972. Tech. Rep. TR-192. Computer Science Center, Univ. of Maryland, College Park, Maryland.

Acta Cryst. (1984). C**40**, 1965–1967

Structure of *N*-[(2β,11bα)-1,3,4,6,7,11b-Hexahydro-2*H*-benzo[*a*]quinolizin-2-yl]-*N*-methyl-1-propanesulphonamide Hydrochloride, WY-26392, $C_{17}H_{26}N_2O_2S.HCl$

BY ALAIN CARPY, ABDESLAM H'NAÏFI AND JEAN-MICHEL LÉGER

Laboratoire de Chimie Analytique, ERA 890, *CNRS, Faculté de Pharmacie, Université de Bordeaux II, Place de la Victoire,* 33076 *Bordeaux CEDEX, France*

(*Received* 8 *June* 1984; *accepted* 20 *July* 1984)

Abstract. α_2-Adrenoceptor antagonist. $M_r = 358{\cdot}94$, monoclinic, $P2_1/c$, $a = 11{\cdot}434$ (1), $b = 14{\cdot}761$ (2), $c = 11{\cdot}800$ (2) Å, $\beta = 113{\cdot}17$ (1)°, $V = 1830{\cdot}9$ (3) Å^3, $Z = 4$, $D_x = 1{\cdot}30$ g cm^{-3}, Cu $K\bar{\alpha}$, $\lambda = 1{\cdot}54178$ Å, $\mu = 29{\cdot}47$ cm^{-1}, $F(000) = 768$, room temperature, $R = 0{\cdot}048$ for 1700 reflections. The protonated endocyclic nitrogen and the sulphonamide group seem to be involved in the binding of the drug to the central α_2-adrenoceptors. The mean bond lengths and angles are as expected. The cohesion of the crystals is ensured by a hydrogen bond between the protonated nitrogen and the Cl^- anion.

Introduction. Among novel substituted benzoquinolizines, WY-26392 exhibits a selective α_2-adrenoceptor antagonist action (Lattimer, Rhodes, Ward, Waterfall & White, 1982). This compound also displays a competitive antagonist activity at 5-HT receptors (McAdams & Rhodes, 1983). Peripherally administered WY-26392 reverses clonidine-induced hypotension in the anaesthetized rat; this result indicates that WY-26392 penetrates into the central nervous system and blocks central α_2-adrenoceptors (Pierce & Shepperson, 1983).

This work is part of a wide conformational analysis among α ligands starting with the agonists (Carpy, Léger, Leclerc, Decker, Rouot & Wermuth, 1982).

Experimental. Small white plates (from ethanol), 0·23 × 0·20 × 0·08 mm, Enraf–Nonius CAD-4 diffractometer with graphite monochromator; 25 reflections ($6 < \theta < 26°$) used to refine orientation matrix; systematic absences: $h0l$ for l odd, $0k0$ for k odd; 2720 ($\pm h,k,l$) independent with $\theta < 60°$, h −12 to +12, k 0 to 16, l 0 to 13; 1700 with $I \geq 3\sigma(I)$; Lp correction, absorption ignored; two check reflections (210, 02$\bar{2}$) every 5400 s showed no unusual variation (all within $\pm 3\sigma$); direct methods, *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980), anisotropic diagonal matrix, refinement on F using observed reflections, $w = 1$ if $|F_o| < P$, $P = (F_{o\,max}^2/10)^{1/2}$, $w = (P/F_o)^2$ if $|F_o| > P$; H from ΔF synthesis,

0108-2701/84/111965-03$01.50

isotropic; $R = 0.048$, $R_w = 0.058$, $S = 0.838$ (1700 reflections, 316 parameters); max. $\Delta\rho$ excursion ± 0.4 e Å^{-3} in final ΔF map; in final cycle mean and max. $\Delta/\sigma = 0.1$ and 0.2; H-atom form factor from Stewart, Davidson & Simpson (1965), all other form factors from *International Tables for X-ray Crystallography* (1974), S atom corrected for anomalous dispersion, Mini 6 CII computer.

Table 1. *Atomic coordinates* ($\times 10^4$) *and equivalent isotropic temperature factors*

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

	x	y	z	B_{eq}(Å^2)
C(1)	−1592 (4)	3742 (3)	10014 (3)	3·0 (1)
C(2)	−865 (4)	4457 (3)	10749 (4)	3·6 (2)
C(3)	−1432 (5)	5102 (3)	1135 (4)	4·3 (2)
C(4)	−2700 (5)	5042 (3)	11009 (4)	4·5 (2)
C(5)	−3417 (4)	4331 (3)	10325 (4)	4·3 (2)
C(6)	−2870 (4)	3679 (3)	9801 (4)	3·5 (2)
C(7)	−3706 (4)	2934 (3)	9037 (4)	4·1 (2)
C(8)	−3135 (4)	2504 (3)	8203 (4)	3·8 (2)
N(9)	−1791 (3)	2258 (2)	8971 (3)	3·0 (1)
C(10)	−973 (4)	3098 (3)	9407 (3)	3·0 (1)
C(11)	368 (4)	2813 (3)	10215 (4)	3·1 (2)
C(12)	920 (4)	2164 (3)	9519 (4)	3·4 (2)
C(13)	57 (4)	1346 (3)	9068 (4)	4·1 (2)
C(14)	−1282 (4)	1650 (3)	8247 (4)	4·2 (2)
N(15)	2233 (3)	1924 (2)	10313 (3)	3·7 (1)
S(16)	3331 (1)	2004 (1)	9773 (1)	4·4 (0)
C(17)	3135 (6)	1041 (4)	8803 (7)	7·3 (3)
C(18)	4165 (8)	1005 (5)	8298 (9)	10·8 (5)
C(19)	4111 (10)	258 (7)	7592 (9)	12·6 (6)
C(20)	2436 (5)	1246 (4)	11291 (5)	5·5 (2)
O(21)	3062 (3)	2780 (2)	9001 (4)	6·1 (2)
O(22)	4518 (3)	1947 (3)	10782 (4)	7·5 (2)
Cl(23)	8425 (1)	1157 (1)	1219 (1)	4·81 (7)

Table 2. *Bond distances* (Å) *and angles* (°)

C(1)–C(2)	1·411 (5)	C(10)–C(11)	1·513 (5)
C(1)–C(6)	1·384 (5)	C(11)–C(12)	1·549 (5)
C(1)–C(10)	1·523 (5)	C(12)–C(13)	1·517 (5)
C(2)–C(3)	1·396 (6)	C(12)–N(15)	1·467 (5)
C(3)–C(4)	1·370 (6)	C(13)–C(14)	1·521 (6)
C(4)–C(5)	1·380 (6)	N(15)–S(16)	1·620 (3)
C(5)–C(6)	1·416 (5)	N(15)–C(20)	1·475 (6)
C(6)–C(7)	1·503 (5)	S(16)–C(17)	1·783 (6)
C(7)–C(8)	1·518 (5)	S(16)–O(21)	1·421 (3)
C(8)–N(9)	1·490 (5)	S(16)–O(22)	1·413 (4)
N(9)–C(10)	1·516 (4)	C(17)–C(18)	1·516 (10)
N(9)–C(14)	1·506 (5)	C(18)–C(19)	1·369 (12)
C(2)–C(1)–C(6)	119·1 (3)	C(10)–C(11)–C(12)	111·2 (3)
C(2)–C(1)–C(10)	119·1 (3)	C(11)–C(12)–C(13)	109·5 (3)
C(6)–C(1)–C(10)	121·7 (3)	C(11)–C(12)–N(15)	109·8 (3)
C(1)–C(2)–C(3)	120·4 (3)	C(13)–C(12)–N(15)	113·2 (3)
C(2)–C(3)–C(4)	120·2 (4)	C(12)–C(13)–C(14)	110·0 (3)
C(3)–C(4)–C(5)	120·2 (2)	N(9)–C(14)–C(13)	109·3 (3)
C(4)–C(5)–C(6)	120·6 (4)	C(12)–N(15)–S(16)	119·2 (2)
C(1)–C(6)–C(5)	119·4 (3)	C(12)–N(15)–C(20)	118·0 (3)
C(1)–C(6)–C(7)	122·3 (3)	S(16)–N(15)–C(20)	116·7 (3)
C(5)–C(6)–C(7)	118·3 (3)	N(15)–S(16)–C(17)	105·9 (2)
C(6)–C(7)–C(8)	111·2 (3)	N(15)–S(16)–O(21)	107·8 (2)
C(7)–C(8)–N(9)	108·1 (3)	N(15)–S(16)–O(22)	107·4 (2)
C(8)–N(9)–C(10)	111·0 (3)	C(17)–S(16)–O(21)	106·9 (2)
C(8)–N(9)–C(14)	109·6 (3)	C(17)–S(16)–O(22)	109·3 (2)
C(10)–N(9)–C(14)	110·9 (3)	O(21)–S(16)–O(22)	118·9 (2)
C(1)–C(10)–N(9)	109·4 (3)	S(16)–C(17)–C(18)	111·1 (4)
C(1)–C(10)–C(11)	114·9 (3)	C(17)–C(18)–C(19)	114·3 (7)
N(9)–C(10)–C(11)	108·9 (3)		

Discussion. Table 1 gives the atomic coordinates and Table 2 the bond distances and angles.* A diagram of the molecule with the atom numbering is shown in Fig. 1.

The six-membered carbon ring (*A*) has a reasonable mean carbon bond length of 1·393 (6) Å and a mean angle of 120·0 (4)°, values ranging from 1·370 to 1·416 Å and from 119·1 to 120·6°. The two Csp^2–Csp^3 bonds are somewhat different: C(6)–C(7) = 1·503 (5) Å and C(1)–C(10) = 1·523 (5) Å. There is a discrepancy between the values of the three N–C bonds within the heterocyclic rings (*B* and *C*): N(9)–C(8) = 1·490 (5) Å < N(9)–C(14) = 1·506 (5) Å < N(9)–C(10) = 1·516 (4) Å. The mean Csp^3–Csp^3 bond distance is 1·524 (5) Å, values ranging from 1·513 to 1·549 Å.

Bond lengths and angles within the sulphonamide group have the expected values. See, for instance, the values obtained in the methanesulphonamide of piperidine-4-spiro-1′-(2′,5′-dioxolane) (Smith-Verdier, García-Blanco & Florencio, 1976). The partial double-bond character of N(15)–S(16) [= 1·620 (3) Å] is explained by an interaction between the lone pair of N(15) and the 3*d* orbitals of S(16). One should notice that the protonated nitrogen of the molecule is N(9).

All other bond distances and angles are normal except C(18)–C(19). The low value obtained for this bond [1·369 (12) Å] is probably due to the high temperature effect at the end of the propyl chain.

Ring *A* plus C(7) and C(10) belong to a single plane; C(8) and N(9) are respectively below [−0·454 (4) Å] and above [0·334 (3) Å] this plane. Ring *C* adopts a chair conformation: N(9) and C(12) being respectively above [0·705 (3) Å] and below [−0·697 (3) Å] the mean plane of atoms C(10),C(11),C(13) and C(14).

The spatial position of S(16) is defined by the torsion angle C(11)–C(12)–N(15)–S(16) = −131 (1)°. The terminal propyl chain is folded, S(16)–C(17)–C(18)–C(19) = 177 (1)°.

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters and mean planes of atoms have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39656 (21 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

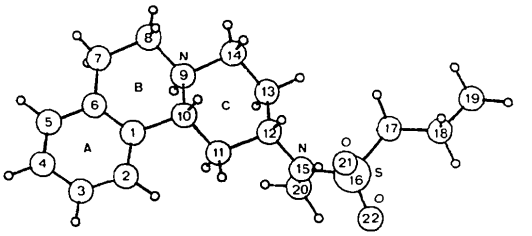

Fig. 1. Perspective view of the molecule showing the numbering of atoms. The bare numbers are for C atoms.

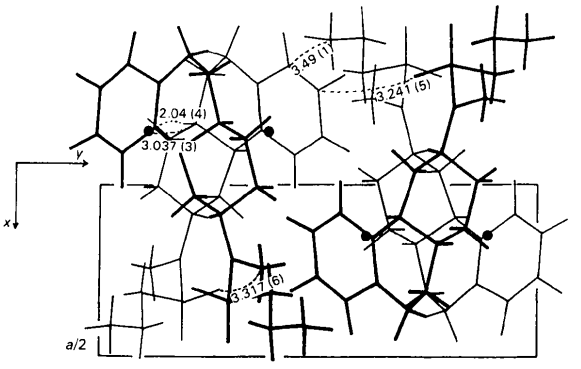

Fig. 2. Packing of molecules projected on (001). (Distances in Å.)

Previous studies on the conformational properties of selective α_1- and α_2-antagonists have shown that there are at least two sites involved in the binding of these drugs to their adrenoceptors: a protonated nitrogen (at physiological pH) and an area rich in electrons (which is in most cases an aromatic system). See, for instance, the structure of WB-4101 {*N*-[2-(2,6-dimethoxyphenoxy)ethyl]-1,4-benzodioxane-2-methylamine} (Carpy, Colleter & Léger, 1981), which is a selective α_1-antagonist, and the structure of BE-2254 {3,4-dihydro-2-[(*p*-hydroxyphenethyl)aminomethyl]-1(2*H*)-naphthalenone} (Carpy, Léger & Colleter, 1984), which is a selective α_2-antagonist. In all cases, the distance between these two sites is close to 5·5 Å. In the present compound, the protonated nitrogen is N(9) and the area rich in electrons is represented by the sulphonamide group. The calculated distance between N(9) and S(16) is 5·57 (1) Å.

The crystalline cohesion is ensured by a hydrogen bond involving $N(9)^+$ and $Cl(23)^-$ ions: N(9)···Cl(23) $(-1+x, y, 1+z) = 3{\cdot}037$ (3) Å, H(109)···Cl(23) = 2·04 (4) Å, N(9)–H(109)···Cl(23) = 177 (3)°, and by van der Waals contacts (Fig. 2).

The authors acknowledge the gift of the sample (Wyeth-Byla, Paris).

References

CARPY, A., COLLETER, J.-C. & LÉGER, J.-M. (1981). *Cryst. Struct. Commun.* **10**, 1391–1395.

CARPY, A., LÉGER, J.-M. & COLLETER, J.-C. (1984). *Acta Cryst.* C**40**, 154–156.

CARPY, A., LÉGER, J.-M., LECLERC, G., DECKER, N., ROUOT, B. & WERMUTH, C. G. (1982). *Mol. Pharmacol.* **21**, 400–408.

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press.

LATTIMER, N., RHODES, K. F., WARD, T. J., WATERFALL, J. F. & WHITE, J. F. (1982). *Br. J. Pharmacol.* **75**, 154 P.

MCADAMS, R. P. & RHODES, K. F. (1983). *Br. J. Pharmacol.* **79**, 308 P.

MAIN, P., FISKE, S. J., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1980). *MULTAN*80. *A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.

PIERCE, V. & SHEPPERSON, N. B. (1983). *Br. J. Pharmacol.* **80**, 463 P.

SMITH-VERDIER, P., GARCÍA-BLANCO, S. & FLORENCIO, F. (1976). *Acta Cryst.* B**32**, 2006–2009.

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

Acta Cryst. (1984). C**40**, 1967–1969

(2,5-Dimethoxy-3-cyclopenten-1-yl)dimethyl(2-propenyl)ammonium Iodide, $C_{12}H_{22}NO_2^+.I^-$

BY ROSEMARIE SWANSON

Chemistry Department, Texas A&M University, College Station, TX 77843, *USA*

AND UNG CHAN YOON AND PATRICK S. MARIANO

Chemistry Department, University of Maryland, College Park, MD 20742, *USA*

(*Received* 20 *September* 1983; *accepted* 20 *July* 1984)

Abstract. $M_r = 339{\cdot}2$, monoclinic, $P2_1/c$, $a = 10{\cdot}233$ (4), $b = 14{\cdot}005$ (8), $c = 11{\cdot}013$ (6) Å, $\beta = 99{\cdot}12$ (4)°, $V = 1558$ (2) Å^3, $Z = 4$, $D_x = 1{\cdot}446$ Mg m^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}71069$ Å, $\mu = 20{\cdot}72$ cm^{-1}, $F(000) = 688$, $T = 297$ K, m.p. = 435–436 K, $R = 0{\cdot}031$, $R_w = 0{\cdot}036$ for 1462 reflections. The molecule, an *N*-allyl-*N*-cyclopentenyldimethylammonium iodide, has two chiral centers in the cyclopentene ring. It is achiral, however, because of an internal plane of symmetry that bisects the cyclopentene π bond. The iodide ion, which lies almost on an extension of the cyclopentene-to-nitrogen bond, has

0108-2701/84/111967-03$01.50