resonance studies (Safe & Moir, 1964). In their studies they made the following assumptions:

(i) the tetrahydroisoquinoline ring is a half-chair;

(ii) the bond joining the two planar moieties is equatorial with respect to the tetrahydroisoquinoline ring;

(iii) the H(1) and H(6′) [or H(1′)] atoms are *gauche*.

For bicuculline (i) is seen to be correct while (ii) and (iii) are incorrect. For narcotine (i) and (ii) are incorrect while (iii) is correct.

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Structure of (+)-7β-Acetyl-3-methoxy-*N*-methyl-6,14-ethenomorphinan-4-ol, $C_{22}H_{27}NO_3$

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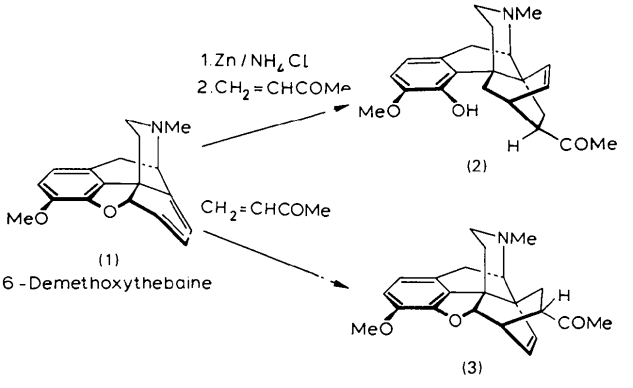
Abstract. $M_r = 353{\cdot}5$, hexagonal, $P6_1$, $a = 11{\cdot}899$ (2), $c = 22{\cdot}478$ (6) Å, $V = 2756{\cdot}2$ Å^3, $Z = 6$, $D_x = 1{\cdot}28$ Mg m^{-3}, λ(Mo $K\alpha$) $= 0{\cdot}71069$ Å, $\mu = 0{\cdot}091$ mm^{-1}, $F(000) = 1140$, $T = 293$ K, final $R = 0{\cdot}033$ for 1707 observed reflections. The acetyl substitutent is in the 7β position of the 6,14-ethenomorphinan skeleton. This means that, when the epoxy ring in 4,5-epoxymorphinan-6,8-dienes has first been opened, the Diels–Alder cycloaddition with methyl vinyl ketone takes place at the other side of the molecule as compared to the addition in morphinan-6,8-dienes with a 4,5-epoxy ring. A novel class of potentially interesting 7β-substituted 6,14-ethenomorphinans becomes herewith available.

Introduction. The title compound (2) was prepared by Diels–Alder reaction of 3-methoxy-*N*-methyl-6,7,8,14-tetradehydromorphinan-4-ol with methyl vinyl ketone. The morphinan-6,8-diene intermediate was obtained by opening of the 4,5-epoxy ring of 6-demethoxythebaine (1) with the aid of zinc and ammonium chloride (Crabbendam, Lie, Linders & Maat, 1984). ^{1}H NMR spectra indicate the cycloaddition takes place in a different way from that observed in 4,5-epoxymorphinans, which yield 6,14-ethenoisomorphinans (3) (van Koningsveld, Maat & Lie, 1984). The structure of (2), however, especially the position of the etheno bridge and that of the acetyl substituent, could not be determined unambiguously from ^{1}H NMR data. Therefore, a single-crystal X-ray analysis was started, which proved the structure of (2) to be (+)-7β-acetyl-3-methoxy-*N*-methyl-6,14-ethenomorphinan-4-ol.



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Experimental. Title compound prepared in the Laboratory of Organic Chemistry starting from 3-methoxy-*N*-methyl-6,7,8,14-tetradehydromorphinan-4-ol and methyl vinyl ketone. Crystals grown from acetone, m.p. 477–478 K, $[\alpha]_D^{25\cdot0°C} = +95°$ [chloroform/ethanol 9:1, 1·1 g dm^{-3}]. D_m not measured. Crystal: approximate dimensions 0·55 × 0·30 × 0·18 mm. CAD-4 diffractometer. Graphite-monochromated Mo $K\alpha$ radiation. Unit cell: 25 reflections, $20\cdot0 < 2\theta < 23\cdot0°$. No absorption corrections. $\theta_{max} = 28°$, $\omega/2\theta$ scan, width = 0·75° + 0·35° tan θ, max. recording time 240 s, $\sigma_{count}(I)/I < 0\cdot02$ requested in a scan. Index range: $0 \le h$, $k \le 13$, $0 \le l \le 29$. Standard reflections 420, $2\bar{6}0$ and $\bar{6}40$: variation <2%. 2271 unique reflections measured, 1712 observed [$I > \sigma(I)$]. Structure solved by *MULTAN* (Germain, Main & Woolfson, 1971). Least-squares refinement minimized $\sum w(\Delta F)^2$, $w = 1$. Refinement in $P6_1$ is consistent with the same absolute configuration for the morphinan skeleton as in previous analyses (van Koningsveld, Lie & Maat, 1984; van Koningsveld, Maat & Lie, 1984). H atoms located from difference Fourier map. Five reflections with high F_c/F_o ratios, possibly due to extinction, removed. Refined parameters included positional parameters of all atoms and anisotropic thermal parameters for heavy atoms; H atoms refined with fixed isotropic temperature factor. $R = 0\cdot033$ for 1707 observed reflections, $S = 0\cdot27$, $(\Delta/\sigma)_{max} = 1\cdot06$ [U_{22} O(3)]. Final ΔF synthesis has $|\rho| < 0\cdot16$ e Å^{-3}. All calculations performed with *XRAY*72 (Stewart, Kruger, Ammon, Dickinson & Hall, 1972).

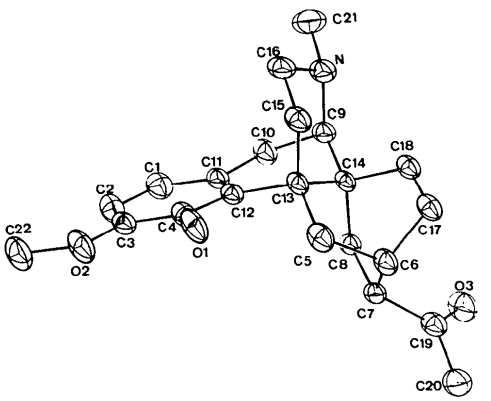

Fig. 1. *ORTEP* plot (Johnson, 1965) of the title compound. Boundary surfaces are drawn to enclose 50% probability.

Table 1. *Final coordinates and equivalent isotropic thermal parameters*

$U_{eq} = \frac{1}{3}(U_{11} + U_{22} + U_{33})$.

	x	y	z	U_{eq}(Å^2)
C(1)	0·3622 (3)	0·0721 (3)	−0·0443 (2)	0·050
C(2)	0·3744 (3)	0·0663 (3)	−0·1054 (1)	0·047
C(3)	0·4005 (3)	−0·0247 (3)	−0·1282 (1)	0·035
C(4)	0·4168 (3)	−0·1090 (3)	−0·0906 (1)	0·034
C(5)	0·5380 (3)	−0·2185 (3)	−0·0067 (1)	0·038
C(6)	0·6309 (3)	−0·1963 (3)	0·0457 (1)	0·038
C(7)	0·6998 (3)	−0·0499 (3)	0·0610 (1)	0·032
C(8)	0·5969 (3)	−0·0147 (3)	0·0785 (1)	0·031
C(9)	0·3552 (3)	−0·1076 (3)	0·0974 (1)	0·036
C(10)	0·3620 (3)	0·0020 (3)	0·0599 (1)	0·044
C(11)	0·3798 (3)	−0·0089 (3)	−0·0063 (1)	0·035
C(12)	0·4122 (3)	−0·0989 (3)	−0·0290 (1)	0·029
C(13)	0·4275 (3)	−0·1924 (2)	0·0125 (1)	0·029
C(14)	0·4597 (3)	−0·1367 (2)	0·0773 (1)	0·028
C(15)	0·2948 (3)	−0·3183 (3)	0·0149 (1)	0·037
C(16)	0·1911 (3)	−0·2942 (3)	0·0397 (1)	0·041
C(17)	0·5532 (3)	−0·2683 (3)	0·0998 (1)	0·037
C(18)	0·4673 (3)	−0·2363 (3)	0·1160 (1)	0·033
C(19)	0·8033 (3)	−0·0175 (3)	0·1078 (1)	0·036
C(20)	0·9165 (4)	−0·0325 (5)	0·0900 (2)	0·065
C(21)	0·1243 (4)	−0·2127 (5)	0·1220 (2)	0·069
C(22)	0·3913 (4)	0·0342 (4)	−0·2290 (2)	0·060
O(1)	0·4345 (2)	−0·2042 (2)	−0·1152*	0·049
O(2)	0·4139 (2)	−0·0433 (2)	−0·1880 (1)	0·053
O(3)	0·7956 (2)	0·0163 (3)	0·1573 (1)	0·058
N	0·2289 (2)	−0·2299 (3)	0·0983 (1)	0·042

* Parameter kept fixed during refinement.

Table 2. *Bond distances* (Å) *and bond angles* (°) *involving non-*H *atoms*

C(1)–C(2)	1·387 (5)	C(9)–C(14)	1·515 (5)
C(1)–C(11)	1·381 (5)	C(9)–N	1·480 (3)
C(2)–C(3)	1·366 (6)	C(10)–C(11)	1·518 (4)
C(3)–C(4)	1·397 (5)	C(11)–C(12)	1·403 (5)
C(3)–O(2)	1·385 (4)	C(12)–C(13)	1·532 (5)
C(4)–O(1)	1·369 (5)	C(13)–C(14)	1·566 (4)
C(4)–C(12)	1·394 (4)	C(13)–C(15)	1·541 (3)
C(5)–C(6)	1·544 (5)	C(14)–C(18)	1·508 (5)
C(5)–C(13)	1·557 (6)	C(15)–C(16)	1·507 (6)
C(6)–C(7)	1·548 (4)	C(16)–N	1·475 (4)
C(6)–C(17)	1·508 (4)	C(17)–C(18)	1·309 (6)
C(7)–C(8)	1·531 (5)	C(19)–O(3)	1·202 (4)
C(7)–C(19)	1·516 (4)	C(19)–C(20)	1·499 (7)
C(8)–C(14)	1·551 (3)	C(21)–N	1·459 (7)
C(9)–C(10)	1·521 (5)	C(22)–O(2)	1·422 (6)

C(2)–C(1)–C(11)	121·4 (4)	C(11)–C(12)–C(13)	120·7 (2)
C(1)–C(2)–C(3)	118·8 (4)	C(5)–C(13)–C(12)	113·3 (2)
C(2)–C(3)–C(4)	120·8 (3)	C(5)–C(13)–C(14)	106·9 (2)
C(2)–C(3)–O(2)	125·4 (3)	C(5)–C(13)–C(15)	111·9 (2)
C(4)–C(3)–O(2)	113·8 (3)	C(12)–C(13)–C(14)	110·6 (2)
C(3)–C(4)–C(12)	120·8 (3)	C(12)–C(13)–C(15)	107·0 (2)
C(3)–C(4)–O(1)	119·0 (3)	C(14)–C(13)–C(15)	107·1 (2)
C(12)–C(4)–O(1)	120·2 (3)	C(8)–C(14)–C(9)	112·4 (2)
C(5) C(6) C(7)	107·0 (3)	C(8) C(14)–C(13)	109·4 (2)
C(5)–C(6)–C(17)	109·6 (2)	C(8)–C(14)–C(18)	106·1 (2)
C(7)–C(6)–C(17)	106·8 (2)	C(9)–C(14)–C(13)	108·6 (2)
C(6)–C(7)–C(8)	108·6 (2)	C(9)–C(14)–C(18)	112·7 (2)
C(6)–C(7)–C(19)	110·3 (3)	C(13)–C(14)–C(18)	107·5 (2)
C(8)–C(7)–C(19)	114·3 (3)	C(13)–C(15)–C(16)	111·5 (3)
C(7)–C(8)–C(14)	110·5 (3)	C(15)–C(16)–N	111·3 (3)
C(10)–C(9)–N	116·3 (3)	C(6)–C(17)–C(18)	113·9 (3)
C(10)–C(9)–C(14)	109·5 (2)	C(14)–C(18)–C(17)	115·5 (2)
C(14)–C(9)–N	109·0 (3)	C(7)–C(19)–C(20)	116·7 (3)
C(9)–C(10)–C(11)	114·8 (3)	C(7)–C(19)–O(3)	122·6 (3)
C(1)–C(11)–C(10)	118·1 (3)	C(20)–C(19)–O(3)	120·7 (3)
C(1)–C(11)–C(12)	120·2 (3)	C(3)–O(2)–C(22)	116·9 (3)
C(10)–C(11)–C(12)	121·7 (3)	C(9)–N–C(16)	113·2 (2)
C(4)–C(12)–C(11)	117·7 (3)	C(9)–N–C(21)	112·7 (3)
C(4)–C(12)–C(13)	121·3 (3)	C(16)–N–C(21)	109·8 (3)

Discussion. The molecular structure is shown in Fig. 1 together with the atom numbering. The final least-

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.

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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, $C_{17}H_{26}N_2O_2S.HCl$

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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,

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