parameters using weights based on counting statistics. The residuals obtained at convergence were $R = 0.043$, $wR = 0.028$ and $S = 2.589$. Weights based on counting statistics were used. The max. $\Delta/\sigma = 0.138$. In the last D map the deepest hole was -0.17 e Å^{-3} and the highest peak 0.21 e Å^{-3}. The secondary-extinction coefficient was 0.35 (2) (Larson, 1967; Zachariasen, 1963). Atomic scattering factors from *NRCVAX*.

Discussion. Table 1* gives the final atomic parameters with their B_{eq} values. Bond lengths and angles are given in Tables 2(*a*) and 2(*b*). Fig. 1 shows the atom numbering and an *ORTEP* perspective view of the tetracyclic compound. The relative stereochemistry found is *trans-syn-cis* as predicted. The structure is relatively rigid; only ring *B* can exist in two conformations, chair and boat, the former being energetically favorable. The observed *trans* and *cis* junctions at C(3)—C(11) and C(10)—C(11) hold ring *C* in a half-chair conformation. No abnormally short intermolecular contacts were observed.

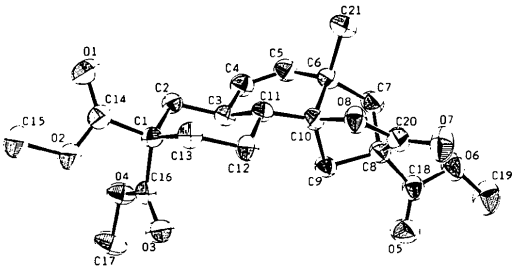

Fig. 1. *ORTEP* (Johnson, 1965) perspective view and crystallographic numbering.

* Lists of structure factors, anisotropic thermal parameters, torsion angles and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53098 (23 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Molecular Structure of Opiate Alkaloids. IV.* Structure of Two Thioniamorphinans

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Abstract. (I) *S*(equatorial)-Allyl-3-hydroxy-17-thioniamorphinan perchlorate, $C_{19}H_{25}OS^+.ClO_4^-$, $M_r = 400.91$, monoclinic, $P2_1/n$, $a = 9.4171$ (8), $b = 10.7425$ (10), $c = 19.096$ (2) Å, $\beta = 95.666$ (7)°, $V = 1922.4$ (3) Å^3, $Z = 4$, $D_x = 1.385$ Mg m^{-3}, λ(Mo $K\alpha$) = 0.70930 Å, $\mu = 0.33$ mm^{-1}, $F(000) = 847.92$, room temperature, final $R = 0.052$ for 1742 observed reflections. (II) *S*(axial)-Allyl-3-hydroxy-17-thioniamorphinan perchlorate, $C_{19}H_{25}OS^+.ClO_4^-$, $M_r = 400.91$, monoclinic, $P2_1$, $a = 8.4554$ (10), $b = 11.658$ (3), $c = 9.5831$ (21) Å, $\beta = 95.620$ (10)°, $V = 940.1$ (3) Å^3, $Z = 2$, $D_x = 1.416$ Mg m^{-3}, λ(Mo $K\alpha$) = 0.70930 Å, $\mu = 0.33$ mm^{-1}, $F(000) = 423.96$, room temperature, final $R = 0.054$ for 1015 observed reflections. The molecular structures of (I) and (II) are differentiated only by the orientation of the *S*-allyl substituent: the *S*-allyl group is equatorial in (I) and axial in (II). It has been shown that the activities as potent and selective blockers of κ opioid

* Part I: Michel, Proulx, Evrard, Norberg & Milchert (1988). Part II: Michel, Evrard, Norberg & Milchert (1988). Part III: Michel & Michel-Dewez (1990).

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receptors ($\kappa 2$ subtype) are to be attributed to the α-thiamorphinan isomer (I). The inactive compound (II) is the β-isomer. The fused ring systems are almost identical in the two molecules.

Introduction. The designs of specific antagonists for the opioid receptors have been largely targeted against μ or δ opioid receptors (Rice, Jacobson, Burke, Bajwa, Streatz & Klee, 1983; Cotton, Giles, Miller, Shaw & Timms, 1984; Hahn, Stzhak, Hishimura, Johnson & Pasternak, 1985). In the third part of the present series (Michel & Michel-Dewez, 1990), we reported a structural study of 19-cyclohexyloripavine analogues, presenting structural elements that would account for the μ and δ receptor specificity (DiMaio, Bayly, Villeneuve & Michel, 1986). It was also important to design specific antagonists for the κ opioid receptors (Portoghese, Lipkowski & Takemori, 1987). Analogues of benzomorphans that specifically block the κ receptor have been developed; more specifically it has also been observed (Belleau, Gulini, Camichioli, Gour-Salin & Sauvé, 1986) that the equatorial form of *S*-allyl-3-hydroxy-17-thioniamorphinan was a potent opioid antagonist. This compound is a morphinan derivative that incorporates a cationic S atom instead of the N atom in position 17 of levallorphan.

The selectivity of these compounds towards the $\kappa 2$ receptor was also reported (Lemaire, Belleau & Jolicoeur, 1989) for endogenous Met-Enk [Arg^6, Phe^7] and dynorphin b.

The present study was undertaken to assign the correct orientation of the *S*-allyl substituent in the active compound. It is unambiguously determined that the active isomer α (I) is equatorial and that the inactive isomer β (II) is axial.

Experimental. Crystals 0·20 × 0·15 × 0·25 mm, from methanol; Enraf–Nonius CAD-4 diffractometer; graphite-monochromated Mo $K\alpha$ radiation; cell parameters were obtained by least-squares procedure on 20 reflections with 2θ in the range 15·00–25·00°. One standard reflection monitored every 100 reflections without significant deviation. The $\omega/2\theta$ scan mode was used for data collection at a constant scan speed of 4° min^{-1}; $2\theta_{max} = 47{\cdot}8°$. Weighting scheme $w = 1/\sigma^2(F)$.

(I) $-9 \le h \le 9$, $0 \le k \le 11$, $0 \le l \le 20$; 2334 unique measured reflections, 1742 observed with $I \ge 2{\cdot}5\sigma(I)$; $R = 0{\cdot}052$, $wR = 0{\cdot}027$; max. Δ/σ (for non-H atoms) $= 0{\cdot}001$; max. and min. densities in final difference map = 0·340 and −0·430 e Å^{-3}.

(II) $-9 \le h \le 9$, $0 \le k \le 13$, $0 \le l \le 10$; 1557 unique measured reflections, 1015 observed with $I \ge 2{\cdot}5\sigma(I)$; $R = 0{\cdot}054$, $wR = 0{\cdot}023$; max. $\Delta/\sigma = 0{\cdot}318$; max. and min. densities in final difference map = 0·280 and −0·290 e Å^{-3}.

Table 1. *Final coordinates and equivalent B values (with e.s.d.'s in parentheses)*

$B_{eq} = (8\pi^2/3)\sum_i\sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	B_{eq} (Å^2)
S(equatorial) isomer				
S	0·85303 (13)	0·69522 (12)	0·13998 (7)	3·71 (6)
O(1)	1·5932 (3)	0·8731 (3)	0·21616 (17)	5·00 (19)
C(1)	1·2011 (5)	0·8543 (4)	0·20568 (22)	2·63 (22)
C(2)	1·3441 (5)	0·8457 (4)	0·23107 (25)	3·2 (3)
C(3)	1·4505 (5)	0·8796 (4)	0·1889 (3)	3·8 (3)
C(4)	1·4158 (6)	0·9213 (5)	0·1212 (3)	4·3 (3)
C(5)	1·2727 (6)	0·9270 (5)	0·0958 (3)	4·0 (3)
C(6)	1·1647 (5)	0·8942 (4)	0·13655 (24)	2·92 (23)
C(7)	1·0130 (5)	0·9065 (5)	0·1037 (3)	3·40 (24)
C(8)	0·9001 (5)	0·8597 (5)	0·1499 (3)	3·5 (3)
C(9)	0·9426 (5)	0·8781 (4)	0·22854 (24)	2·95 (24)
C(10)	0·9458 (5)	1·0159 (4)	0·2459 (3)	3·7 (3)
C(11)	0·9856 (7)	1·0349 (5)	0·3250 (3)	4·5 (3)
C(12)	1·1282 (6)	0·9725 (5)	0·3484 (3)	4·1 (3)
C(13)	1·1217 (5)	0·8356 (5)	0·3298 (3)	3·6 (3)
C(14)	1·0861 (4)	0·8113 (4)	0·25078 (22)	2·81 (22)
C(15)	1·0667 (5)	0·6694 (4)	0·2422 (3)	3·6 (3)
C(16)	1·0242 (5)	0·6274 (4)	0·1676 (3)	3·9 (3)
C(17)	0·8234 (7)	0·6638 (6)	0·0465 (3)	5·1 (3)
C(18)	0·7041 (10)	0·7383 (9)	0·0150 (4)	8·6 (5)
C(19)	0·5849 (14)	0·7219 (12)	0·0067 (5)	12·6 (8)
Cl	0·65391 (17)	0·77613 (15)	0·41545 (8)	5·27 (8)
O(2)	0·6655 (4)	0·8571 (4)	0·35810 (20)	8·6 (3)
O(3)	0·6871 (5)	0·8403 (4)	0·47852 (21)	10·6 (3)
O(4)	0·5097 (4)	0·7335 (4)	0·41165 (23)	10·0 (3)
O(5)	0·7436 (4)	0·6732 (4)	0·41050 (22)	9·5 (3)
S(axial) isomer				
Cl	0·2319 (4)	0	0·2190 (3)	4·22 (15)
S	0·2377 (3)	0·4041 (3)	0·6205 (3)	3·61 (14)
C(1)	0·6519 (11)	0·3060 (9)	0·6973 (9)	2·5 (5)
C(2)	0·7526 (12)	0·2117 (9)	0·6878 (11)	3·2 (5)
C(3)	0·8442 (12)	0·1997 (10)	0·5780 (10)	3·2 (5)
C(4)	0·8346 (14)	0·2819 (12)	0·4724 (11)	4·1 (6)
C(5)	0·7364 (13)	0·3753 (13)	0·4790 (10)	4·4 (6)
C(6)	0·6413 (11)	0·3884 (9)	0·5891 (9)	3·0 (5)
C(7)	0·5337 (16)	0·4904 (12)	0·5883 (13)	4·4 (7)
C(8)	0·4109 (12)	0·4845 (10)	0·6963 (10)	3·0 (5)
C(9)	0·4863 (12)	0·4384 (8)	0·8332 (10)	2·6 (5)
C(10)	0·6183 (13)	0·5150 (10)	0·8990 (12)	3·3 (6)
C(11)	0·6973 (13)	0·4709 (11)	1·0351 (13)	4·1 (6)
C(12)	0·7587 (12)	0·3496 (12)	1·0190 (10)	3·7 (6)
C(13)	0·6241 (14)	0·2721 (11)	0·9617 (11)	3·5 (6)
C(14)	0·5436 (12)	0·3137 (9)	0·8163 (10)	2·9 (5)
C(15)	0·4034 (13)	0·2316 (10)	0·7768 (11)	3·0 (5)
C(16)	0·3107 (15)	0·2593 (10)	0·6359 (12)	3·5 (5)
C(17)	0·1002 (13)	0·4140 (12)	0·7534 (11)	3·6 (6)
C(18)	0·0408 (12)	0·5325 (10)	0·7729 (14)	3·7 (6)
C(19)	0·0547 (15)	0·5792 (11)	0·8951 (14)	5·0 (7)
O(1)	0·9446 (8)	0·1088 (7)	0·5741 (7)	4·3 (4)
O(2)	0·2160 (9)	0·3187 (8)	0·0827 (7)	5·9 (5)
O(3)	0·3629 (11)	0·4289 (11)	0·2480 (12)	11·4 (7)
O(4)	0·2294 (17)	0·2673 (9)	0·3116 (9)	12·0 (9)
O(5)	0·0981 (10)	0·4287 (8)	0·2420 (8)	7·2 (5)

No correction was made for absorption; 53 standard reflections, 2% intensity variation. The *NRCVAX* system was used for all calculations (Gabe, Lee & Le Page, 1985). The structures were solved by the application of direct methods and refined for full-matrix least squares on *F*. Anisotropic thermal parameters were refined for non-H atoms. The H atoms were located from a difference map and refined with isotropic thermal factors. Atomic scattering factors from *NRCVAX*.

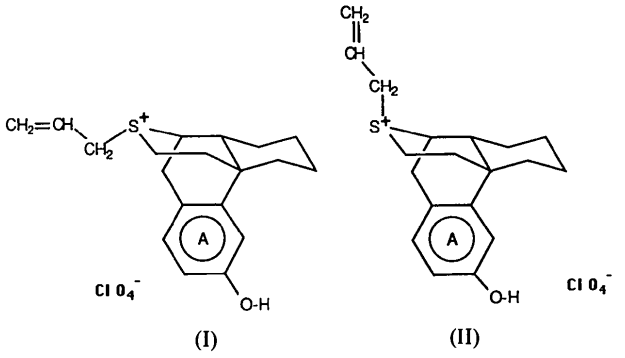
The absolute configuration was determined from the effects of anomalous dispersion from the S atom on 20 Friedel pairs of reflections (Bijvoet, Peerdeman & Van Bommel, 1951). The η (Rogers, 1981) parameter for the presented enantiomer was refined to be +0·96 (5).

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

	S(axial) isomer	*S*(equatorial) isomer		*S*(axial) isomer	*S*(equatorial) isomer
S—C(8)	1·828 (11)	1·827 (5)	C(9)—C(10)	1·518 (15)	1·517 (7)
S—C(16)	1·798 (12)	1·800 (5)	C(9)—C(14)	1·545 (14)	1·553 (6)
S—C(17)	1·810 (10)	1·812 (6)	C(10)—C(11)	1·496 (17)	1·553 (8)
O(1)—C(3)	1·360 (13)	1·394 (6)	C(11)—C(12)	1·520 (18)	1·528 (8)
C(1)—C(2)	1·399 (14)	1·388 (6)	C(12)—C(13)	1·514 (17)	1·513 (8)
C(1)—C(6)	1·410 (14)	1·398 (6)	C(13)—C(14)	1·567 (14)	1·535 (6)
C(1)—C(14)	1·533 (13)	1·521 (6)	C(14)—C(15)	1·542 (15)	1·542 (7)
C(2)—C(3)	1·374 (14)	1·394 (7)	C(15)—C(16)	1·528 (15)	1·511 (8)
C(3)—C(4)	1·391 (17)	1·378 (8)	C(17)—C(18)	1·488 (18)	1·459 (10)
C(4)—C(5)	1·374 (19)	1·387 (8)	C(18)—C(19)	1·287 (19)	1·132 (16)
C(5)—C(6)	1·396 (13)	1·387 (7)	Cl—O(2)	1·384 (7)	1·411 (4)
C(6)—C(7)	1·497 (17)	1·508 (7)	Cl—O(3)	1·379 (10)	1·396 (4)
C(7)—C(8)	1·538 (15)	1·532 (7)	Cl—O(4)	1·392 (10)	1·428 (4)
C(8)—C(9)	1·510 (14)	1·529 (7)	Cl—O(5)	1·426 (9)	1·400 (4)
C(8)—S—C(16)	101·2 (5)	99·20 (21)	C(10)—C(9)—C(14)	111·8 (8)	113·2 (4)
C(8)—S—C(17)	103·4 (5)	107·1 (3)	C(9)—C(10)—C(11)	114·0 (10)	110·1 (4)
C(16)—S—C(17)	104·0 (6)	105·0 (3)	C(10)—C(11)—C(12)	111·1 (9)	110·6 (4)
C(2)—C(1)—C(6)	118·9 (8)	119·3 (4)	C(11)—C(12)—C(13)	109·9 (9)	110·2 (4)
C(2)—C(1)—C(14)	120·4 (9)	120·1 (4)	C(12)—C(13)—C(14)	112·6 (9)	113·3 (4)
C(6)—C(1)—C(14)	120·5 (9)	120·4 (4)	C(1)—C(14)—C(9)	110·5 (8)	110·7 (3)
C(1)—C(2)—C(3)	121·5 (10)	120·6 (4)	C(1)—C(14)—C(13)	113·9 (8)	114·0 (4)
O(1)—C(3)—C(2)	120·0 (10)	119·5 (5)	C(1)—C(14)—C(15)	106·3 (8)	108·9 (4)
O(1)—C(3)—C(4)	120·7 (9)	119·8 (4)	C(9)—C(14)—C(13)	108·2 (8)	106·9 (4)
C(2)—C(3)—C(4)	119·3 (10)	120·6 (4)	C(9)—C(14)—C(15)	111·6 (9)	109·7 (3)
C(3)—C(4)—C(5)	120·4 (10)	118·4 (5)	C(13)—C(14)—C(15)	106·4 (8)	106·5 (4)
C(4)—C(5)—C(6)	121·1 (11)	122·2 (5)	C(14)—C(15)—C(16)	113·7 (9)	114·4 (4)
C(1)—C(6)—C(5)	118·8 (10)	118·9 (4)	S—C(16)—C(15)	114·4 (8)	107·6 (3)
C(1)—C(6)—C(7)	122·7 (8)	123·7 (4)	S—C(17)—C(18)	113·3 (9)	109·9 (5)
C(5)—C(6)—C(7)	118·6 (10)	117·4 (4)	C(17)—C(18)—C(19)	120·3 (11)	133·2 (11)
C(6)—C(7)—C(8)	114·3 (10)	114·5 (4)	O(2)—Cl—O(3)	113·2 (6)	109·7 (3)
S—C(8)—C(7)	108·9 (8)	115·7 (4)	O(2)—Cl—O(4)	109·4 (5)	107·7 (3)
S—C(8)—C(9)	114·8 (7)	105·3 (3)	O(2)—Cl—O(5)	109·5 (5)	109·9 (3)
C(7)—C(8)—C(9)	110·3 (9)	113·2 (4)	O(3)—Cl—O(4)	112·8 (8)	109·5 (3)
C(8)—C(9)—C(10)	112·6 (9)	109·8 (4)	O(3)—Cl—O(5)	105·5 (6)	111·3 (3)
C(8)—C(9)—C(14)	110·8 (8)	110·2 (4)	O(4)—Cl—O(5)	106·0 (7)	108·7 (3)

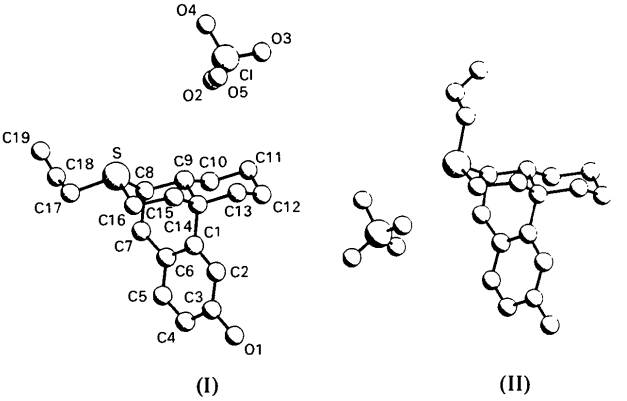
Discussion. Final atomic parameters are given in Table 1.* Bond lengths and valence angles are given in Table 2. Fig. 1 shows the molecular schemes for (I) and (II). Perspective views of both title compounds are depicted in Fig. 2. The results of the structure determination indicate that (I) and (II) have identical geometries for the fused-ring system. Compound (I) is clearly the equatorial and compound (II) the axial *S*-allyl isomer. No significant distortion in the ring system is induced by this differentiation. Following the synthetic pathway, racemic mixtures were expected for both compounds. Nevertheless, the *S*-allyl (axial) compound (II) was found to crystallize in the polar $P2_1$ space group. The separation of stereoisomers is achieved by the recrystallization. No abnormally short intermolecular contacts were noted in the crystal packing. The lack of a

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53101 (23 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.



(I) (II)

Fig. 1. Molecular schemes.



(I) (II)

Fig. 2. *PLUTO* (Motherwell & Clegg, 1978) perspective view and atom numbering for both title compounds.

potential acceptor explains the fact that the OH group is not involved in a hydrogen bond.

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Structure of an Aspirin Derivative: 2-(2-Methoxybenzyloxy)-2-methyl-4*H*-1,3-benzodioxin-4-one

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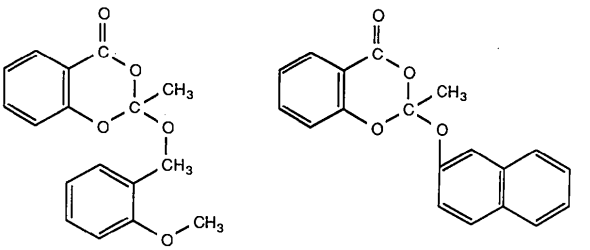
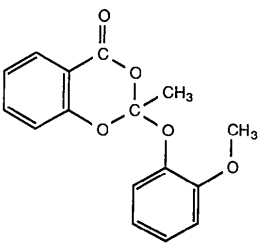
Abstract. $C_{17}H_{16}O_5$, $M_r = 300{\cdot}31$, monoclinic, $P2_1/n$, $a = 14{\cdot}196\ (2)$, $b = 10{\cdot}131\ (1)$, $c = 10{\cdot}601\ (1)$ Å, $\beta = 104{\cdot}658\ (7)°$, $V = 1475{\cdot}0\ (3)$ Å^3, $Z = 4$, $D_x = 1{\cdot}352$ g cm^{-3}, λ(Mo $K\alpha$) $= 0{\cdot}71073$ Å, $\mu = 0{\cdot}9075$ cm^{-1}, $F(000) = 632$, $T = 295$ K, $R = 0{\cdot}056$, $wR = 0{\cdot}071$ for 1052 unique reflections ($I > 3\sigma$) and 200 variables. The title compound (I) is a cyclic ortho ester derivative of aspirin. The dioxane ring of the aspirin moiety is in a half-boat conformation, the 2-methoxybenzyloxy group is axial to this ring. The structure of (I) shows similarities to those of two other cyclic ortho ester aspirin derivatives, 2-methyl-2-(2-naphthyloxy)-(II) and 2-(2-methoxyphenoxy)-2-methyl-4*H*-1,3-benzodioxin-4-one (III).

Introduction. Aspirin (IV) is in common clinical use, but unfortunately it has several bad qualities such as a relatively narrow therapeutic margin, it irritates the gastric mucosa, and it hydrolyses relatively quickly to salicylic acid (V). Therefore, various attempts have been made to design prodrugs for aspirin which do not have the mentioned undesirable effects (Hansen & Senning, 1983). (The term *prodrug* refers to a compound which will act as a precursor of a particular drug when administered to an organism.) The chemical structure of the title compound (I) and two other cyclic ortho ester aspirin derivatives whose crystal structures are known by X-ray analysis, (II) (Jørgensen & Hansen, 1982) and (III) (Destro &



(I)

(II)



(III)

Saccarello, 1983), can be generalized as (VI). This type of ortho ester will undergo hydrolysis according to the scheme below, which shows model pathways

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