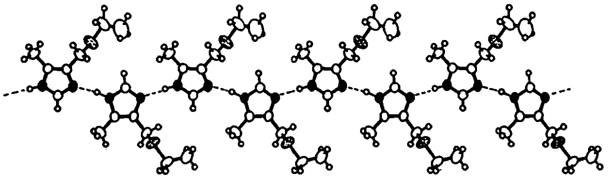

Fig. 2. Molecules of 4-(ethylthiomethyl)-5-methylimidazole linked by hydrogen bonds along the *a* axis.

plane through N(11)—C(12)—N(13)—C(14)—C(15) and the plane through C(10)—S(19)—C(18) make an angle of 103·9 (2)° with one another, while the imidazole plane through N(21)—C(22)—N(23)—C(24)—C(25) and the plane through C(20)—S(29)—C(28) make an angle of 87·1(3)° with one another. The angles formed by the corresponding planes in the coordinated ligand are also close to 90°. In [Co(memi)$_2$(NCS)$_2$] this angle is 91·6 (1)°, in [Ni(memi)$_2$(H$_2$O)$_2$](NO$_3$)$_2$ it is 90·3 (2)° and in [Cu(memi)$_2$(H$_2$O)$_2$](NO)$_2$ it is 86·5 (3)° (Bouwman, Westheide, Driessen & Reedijk, 1989). The conformations of the free ligand and the coordinated ligand are thus hardly different. This means that the conformation of the free ligand is favorable for coordination.

There is no intermolecular stacking of the aromatic rings. The packing of the molecules is dictated by normal van der Waals contacts and the hydrogen bonding noted above.

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Structure of Strychnine Hydrochloride Sesquihydrate

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Abstract. $C_{21}H_{23}N_2O_2^+.Cl^-.1\cdot5H_2O$, $M_r = 397\cdot90$, monoclinic, $P2_1$, $a = 7\cdot617$ (1), $b = 32\cdot463$ (2), $c = 7\cdot849$ (1) Å, $\beta = 90\cdot40$ (2)°, $V = 1940\cdot8$ (4) Å^3, $Z = 4$, $D_m = 1\cdot39$, $D_x = 1\cdot36$ g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 19\cdot724$ cm^{-1}, $F(000) = 844$, final $R = 0\cdot047$ for 3368 observed reflections. Strychnine hydrochloride is a naturally occurring alkaloid in its protonated form. One of the N atoms accepts the proton from hydrochloric acid changing its hybridization to sp^3. The indole N atom is sp^2 hybridized with its lone-

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pair electron involved in conjugation with the carbonyl group. The hydrogen bonds form a complex zigzag network which stabilizes the structure.

Introduction. Strychnine is a naturally occurring alkaloid and is isolated from the seeds of *Strychnos nuxvomica* L. The importance of a precise structure and conformation analysis of the molecule arises from its neuromuscular blocking action (Manske & Holmes, 1950). The present crystal structure determination was undertaken to gain some understanding of the molecular conformation of this neuromuscular blocking agent in its protonated form and to deduce the packing arrangement of the molecules in the crystal lattice.

Experimental. Colourless needle-shaped crystals (from ethanol); density by flotation in benzene–bromoform; crystal size 0·25 × 0·40 × 0·20 mm; $P2_1$ (systematic absences: $0k0$, k odd); PW1100 computer-controlled single-crystal X-ray diffractometer; graphite-monochromated Cu $K\alpha$ radiation; cell parameters from 25 reflections $35 < 2\theta < 50°$, 3420 unique reflections $(\sin\theta/\lambda)_{\max} = 0{\cdot}634$ Å^{-1} $(-9 \le h \le 9,\ 0 \le k \le 40,\ 0 \le l \le 7)$, 3368 observed reflections $[I \ge 2{\cdot}5\sigma(I)]$; intensities corrected for Lp, absorption ignored; $\omega/2\theta$ scan mode, scan speed variable, three standard reflections monitored after every hour of X-ray exposure; structure solved by heavy-atom method. Non-H atoms were located from successive Fourier syntheses; full-matrix least-squares refinement of the non-H atoms based on F with anisotropic thermal parameters (*SHELX76*; Sheldrick, 1976); all H atoms, except one attached to the water O(3) atom, located from difference synthesis but not refined, $R = 0{\cdot}048$, unit weights, $\Delta/\sigma < 0{\cdot}15$, $S = 1{\cdot}95$, maximum residual $\Delta\rho = 0{\cdot}35$ e Å^{-3} in final difference synthesis, scattering factors from *International Tables for X-ray Crystallography* (1974). The atomic coordinates of non-H atoms are listed in Table 1,* and bond lengths and bond angles are given in Table 2.

Table 1. *Fractional coordinates of non-*H *atoms with e.s.d.'s in parentheses and equivalent isotropic thermal parameters* (Å^2)

$$U_{\rm eq} = \tfrac{1}{3}\textstyle\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
Molecule *A*				
O(1)	0·3326 (6)	0·7519 (1)	−0·0905 (6)	0·0617
O(2)	0·1200 (5)	0·8465 (1)	−0·1932 (5)	0·0489
N(1)	0·2852 (5)	0·8109 (1)	0·0594 (5)	0·0338
N(2)	0·0238 (5)	0·9190 (1)	0·3414 (6)	0·0390
C(1)	0·3418 (6)	0·8289 (2)	0·3379 (7)	0·0381
C(2)	0·4194 (7)	0·8257 (2)	0·4973 (7)	0·0499
C(3)	0·5354 (8)	0·7929 (2)	0·5258 (9)	0·0544
C(4)	0·5730 (7)	0·7660 (2)	0·4012 (10)	0·0579
C(5)	0·4987 (7)	0·7689 (2)	0·2350 (8)	0·0494
C(6)	0·3809 (6)	0·8013 (1)	0·2100 (7)	0·0356
C(7)	0·1556 (6)	0·8440 (1)	0·0984 (6)	0·0297
C(8)	0·2195 (6)	0·8625 (1)	0·2710 (6)	0·0313
C(9)	0·0695 (6)	0·8746 (2)	0·3921 (6)	0·0350
C(10)	−0·0922 (6)	0·8478 (2)	0·3859 (6)	0·0388
C(11)	−0·1609 (6)	0·8467 (2)	0·2016 (6)	0·0339
C(12)	−0·0261 (6)	0·8283 (1)	0·0979 (6)	0·0299
C(13)	−0·0716 (7)	0·8120 (2)	−0·0890 (6)	0·0373
C(14)	0·0909 (8)	0·7939 (2)	−0·1789 (7)	0·0495
C(15)	0·2452 (7)	0·7829 (2)	−0·0679 (7)	0·0420
C(16)	−0·2837 (8)	0·8657 (2)	−0·1431 (7)	0·0572
C(17)	−0·2505 (7)	0·8998 (2)	−0·0175 (8)	0·0464
C(18)	−0·1935 (6)	0·8903 (2)	0·1407 (7)	0·0366
C(19)	−0·1596 (7)	0·9239 (2)	0·2680 (7)	0·0421
C(20)	0·1661 (7)	0·9343 (2)	0·2228 (7)	0·0440
C(21)	0·3155 (6)	0·9038 (1)	0·2480 (7)	0·0397
Molecule *B*				
O(1)	0·1743 (6)	0·2198 (1)	0·2616 (6)	0·0607
O(2)	0·6208 (6)	0·1241 (1)	0·1668 (5)	0·0452
N(1)	0·2161 (6)	0·1612 (1)	0·4127 (6)	0·0335
N(2)	0·4678 (6)	0·0514 (1)	0·6970 (6)	0·0397
C(1)	0·1574 (7)	0·1427 (2)	0·6905 (7)	0·0350
C(2)	0·0792 (7)	0·1465 (2)	0·8473 (8)	0·0461
C(3)	−0·0380 (8)	0·1791 (2)	0·8770 (9)	0·0551
C(4)	−0·0752 (8)	0·2066 (2)	0·7452 (9)	0·0550
C(5)	0·0001 (8)	0·2030 (2)	0·5845 (9)	0·0475
C(6)	0·1207 (7)	0·1706 (2)	0·5612 (7)	0·0358
C(7)	0·3443 (6)	0·1275 (1)	0·4534 (7)	0·0280
C(8)	0·2778 (7)	0·1095 (2)	0·6254 (7)	0·0304
C(9)	0·4267 (7)	0·0960 (2)	0·7483 (7)	0·0358
C(10)	0·5905 (7)	0·1224 (2)	0·7435 (7)	0·0384
C(11)	0·6585 (7)	0·1233 (2)	0·5616 (7)	0·0324
C(12)	0·5251 (6)	0·1475 (1)	0·4550 (6)	0·0287
C(13)	0·5713 (7)	0·1582 (2)	0·2694 (7)	0·0359
C(14)	0·4101 (8)	0·1757 (2)	0·1762 (8)	0·0460
C(15)	0·2568 (7)	0·1880 (2)	0·2857 (7)	0·0396
C(16)	0·7812 (8)	0·1040 (2)	0·2174 (8)	0·0529
C(17)	0·7447 (8)	0·0701 (2)	0·3435 (8)	0·0462
C(18)	0·6886 (6)	0·0791 (2)	0·4994 (7)	0·0361
C(19)	0·6494 (8)	0·0461 (2)	0·6251 (8)	0·0454
C(20)	0·3284 (8)	0·0370 (2)	0·5724 (8)	0·0456
C(21)	0·1793 (8)	0·0682 (2)	0·5976 (8)	0·0420
Non-bonded atoms				
Cl(1)	0·0150 (2)	−0·4641 (1)	0·3293 (2)	0·0612
Cl(2)	0·4955 (2)	−0·0005 (1)	0·0222 (2)	0·0586
O(3)	0·1921 (7)	0·0614 (2)	0·1320 (7)	0·0748
O(4)	0·0916 (6)	0·5156 (2)	0·0006 (7)	0·0733
O(5)	0·3407 (9)	0·9205 (2)	0·7865 (10)	0·1188

Discussion. Fig. 1 shows the atom-labelling scheme; the seven rings constituting the strychnine molecule are numbered I to VII. In each asymmetric unit, the present structure contains two crystallographically independent protonated strychnine molecules, two chloride counter ions, and three molecules of water. The independent molecules in the asymmetric unit are designated *A* and *B* for convenience.

The phenyl ring (I) is planar while ring II assumes a twist conformation, which is evident from the puckering coordinates (Cremer & Pople, 1975). The twist axis passes through C(6) in each molecule. The endocyclic angles in ring I at C(4), C(5) and C(6) deviate from the average value by 2·2, −4·2 and 2·0° in molecule *A*, and 2·4, −4·1 and 1·8° in molecule *B*, respectively. The average bond length in ring I is 1·389 (8) Å. The distribution of the aromatic bond

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* Lists of coordinates of H atoms, anisotropic thermal parameters, bond distances and angles involving H atoms, torsion angles, least-squares planes, puckering parameters, and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52017 (36 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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

	A	*B*		*A*	*B*
O(1)—C(15)	1·220 (7)	1·223 (7)	C(7)—C(8)	1·557 (6)	1·559 (8)
O(2)—C(13)	1·433 (7)	1·421 (7)	C(7)—C(12)	1·538 (6)	1·522 (6)
O(2)—C(16)	1·451 (7)	1·439 (7)	C(8)—C(9)	1·542 (7)	1·547 (8)
N(1)—C(6)	1·419 (6)	1·411 (7)	C(8)—C(21)	1·538 (5)	1·551 (9)
N(1)—C(7)	1·492 (5)	1·499 (6)	C(9)—C(10)	1·508 (7)	1·514 (8)
N(1)—C(15)	1·383 (7)	1·360 (7)	C(10)—C(11)	1·535 (7)	1·522 (8)
N(2)—C(9)	1·535 (7)	1·536 (7)	C(11)—C(12)	1·518 (7)	1·529 (7)
N(2)—C(19)	1·516 (7)	1·507 (8)	C(11)—C(18)	1·514 (9)	1·533 (9)
N(2)—C(20)	1·517 (7)	1·513 (8)	C(12)—C(13)	1·549 (7)	1·541 (7)
C(1)—C(2)	1·384 (8)	1·377 (8)	C(13)—C(14)	1·545 (8)	1·534 (8)
C(1)—C(6)	1·380 (7)	1·387 (8)	C(14)—C(15)	1·501 (8)	1·508 (8)
C(1)—C(8)	1·525 (7)	1·507 (8)	C(16)—C(17)	1·503 (9)	1·507 (9)
C(2)—C(3)	1·401 (9)	1·405 (9)	C(17)—C(18)	1·348 (8)	1·331 (8)
C(3)—C(4)	1·343 (10)	1·394 (10)	C(18)—C(19)	1·500 (8)	1·488 (9)
C(4)—C(5)	1·421 (10)	1·394 (10)	C(20)—C(21)	1·520 (7)	1·536 (9)
C(5)—C(6)	1·395 (7)	1·409 (9)			

	A	*B*		*A*	*B*
C(13)—O(2)—C(16)	113·5 (4)	115·1 (4)	O(1)—C(15)—N(1)	122·0 (5)	122·3 (5)
C(6)—N(1)—C(7)	108·9 (3)	108·7 (4)	O(1)—C(15)—C(14)	122·5 (5)	122·3 (6)
C(6)—N(1)—C(15)	124·5 (4)	126·0 (5)	N(1)—C(15)—C(14)	115·5 (5)	115·4 (5)
C(7)—N(1)—C(15)	118·6 (4)	118·1 (4)	O(2)—C(16)—C(17)	110·7 (5)	110·6 (5)
C(9)—N(2)—C(19)	113·8 (4)	113·3 (5)	C(16)—C(17)—C(18)	119·2 (6)	120·3 (6)
C(9)—N(2)—C(20)	107·8 (4)	108·5 (5)	C(11)—C(18)—C(17)	123·8 (6)	123·2 (6)
C(19)—N(2)—C(20)	113·1 (4)	111·4 (5)	C(1)—C(6)—C(5)	121·9 (5)	121·4 (5)
C(2)—C(1)—C(6)	121·1 (5)	120·6 (5)	N(1)—C(7)—C(8)	104·7 (3)	104·1 (3)
C(2)—C(1)—C(8)	128·4 (5)	129·5 (5)	N(1)—C(7)—C(12)	106·3 (3)	106·2 (3)
C(6)—C(1)—C(8)	110·4 (4)	109·8 (5)	C(8)—C(7)—C(12)	116·5 (4)	116·9 (4)
C(1)—C(2)—C(3)	117·8 (6)	119·7 (6)	C(1)—C(8)—C(7)	102·1 (3)	103·2 (4)
C(2)—C(3)—C(4)	121·0 (6)	119·0 (6)	C(1)—C(8)—C(9)	115·0 (4)	115·9 (5)
C(3)—C(4)—C(5)	122·6 (6)	122·3 (6)	C(1)—C(8)—C(21)	112·0 (4)	111·8 (5)
C(4)—C(5)—C(6)	115·5 (5)	116·9 (6)	C(7)—C(8)—C(9)	114·0 (4)	113·9 (4)
N(1)—C(6)—C(1)	110·6 (4)	111·1 (5)	C(7)—C(8)—C(21)	112·3 (4)	111·2 (4)
N(1)—C(6)—C(5)	127·5 (5)	127·5 (5)	C(9)—C(8)—C(21)	101·8 (3)	101·2 (5)
C(10)—C(11)—C(12)	106·8 (4)	107·1 (4)	C(11)—C(18)—C(19)	116·2 (5)	115·6 (5)
C(10)—C(11)—C(18)	109·3 (4)	109·5 (5)	C(17)—C(18)—C(19)	120·0 (6)	121·2 (6)
C(12)—C(11)—C(18)	114·1 (4)	114·0 (4)	N(2)—C(19)—C(18)	109·3 (4)	110·8 (5)
C(7)—C(12)—C(11)	113·1 (4)	112·5 (4)	N(2)—C(20)—C(21)	104·1 (4)	103·3 (5)
C(7)—C(12)—C(13)	107·5 (4)	107·5 (4)	C(8)—C(21)—C(20)	103·1 (3)	103·3 (5)
C(11)—C(12)—C(13)	118·6 (4)	118·5 (4)	N(2)—C(9)—C(8)	104·3 (4)	104·7 (5)
O(2)—C(13)—C(12)	114·2 (5)	115·0 (5)	N(2)—C(9)—C(10)	110·5 (4)	110·9 (5)
O(2)—C(13)—C(14)	103·9 (4)	103·5 (5)	C(8)—C(9)—C(10)	116·2 (4)	115·1 (5)
C(12)—C(13)—C(14)	110·4 (4)	110·3 (4)	C(9)—C(10)—C(11)	108·5 (4)	108·7 (5)
C(13)—C(14)—C(15)	116·9 (5)	116·5 (5)			

lengths in both molecules is in good agreement with those calculated for similar structures. The angles around N(1) in both molecules *A* and *B* are in good agreement with the corresponding values for strychnine sulfonic acid tetrahydrate (Sake Gowda, Cartz & Natarajan, 1973).

The six-membered ring III is nonplanar in both molecules. The angular strain in this ring is shown by the deviation of the bond angles in the ring from the sp^3 value. In each molecule this ring exhibits a distorted 'chair' conformation (Cremer & Pople, 1975). The C(10), C(11), C(18) and C(19) atoms of ring IV are coplanar in both *A* and *B*, as indicated by the torsion angle C(10)—C(11)—C(18)—C(19) [−1·88 (65) and −0·86 (53)° in *A* and *B*, respectively]. The ring is in a 'boat' conformation (Cremer & Pople, 1975). The puckering parameters of the five-membered ring V in either molecule suggest that the rings assume one of the ten 'twist' conformations with the twist axis through N(2) in both molecules (Cremer & Pople, 1975). For the seven-membered ring VI in both molecules, the torsion angle C(11)—C(18)—C(17)—C(16) [−0·30 (88) and −0·33 (19)°] shows that these atoms are planar. However, the other torsion angles reveal the nonplanarity of the rings in both molecules. The conformation of the six-membered ring VII tends to show one of the six 'twist-boat' conformations in both molecules (Cremer & Pople, 1975). The O(1) atom lies nearly *cis* to C(6) as indicated by the torsion angle C(6)—N(1)—C(15)—O(1) [−24·20 (80) and −21·61 (88)° in molecules *A* and *B*, respectively]. The tricovalent N(1) atom has a free electron pair which has a tendency to be coplanar with the π-electronic system of the aromatic ring. The double-bond nature of C(15)—O(1) is decreased resulting in the lengthening of this bond. On the other hand, the shortening of N(1)—C(15) suggests a decrease in its single-bond character. These deviations from standard values may be attributed to the conjugation of N(1) with the carbonyl group C(15)=O(1) (Banerjee & Chaudhuri, 1986), but the bond lengths are in good agreement with those in strychnine sulfonic acid tetrahydrate (Sake Gowda, Cartz & Natarajan, 1973). The N(2) atom accepts the proton from hydrochloric acid changing its hybridization to sp^3.

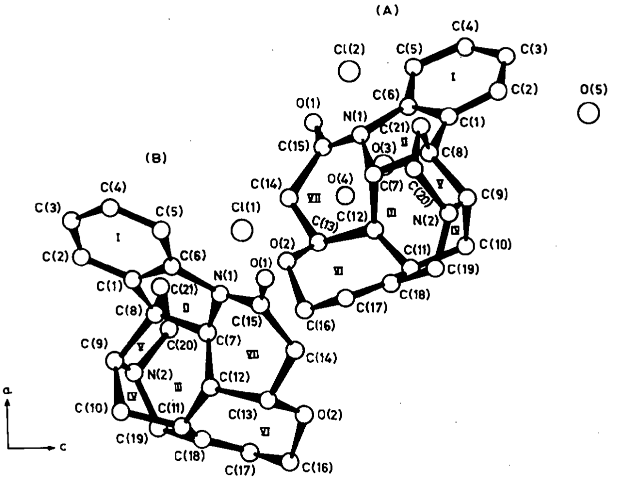

Fig. 1. A view of strychnine hydrochloride sesquihydrate with the atom-numbering scheme.

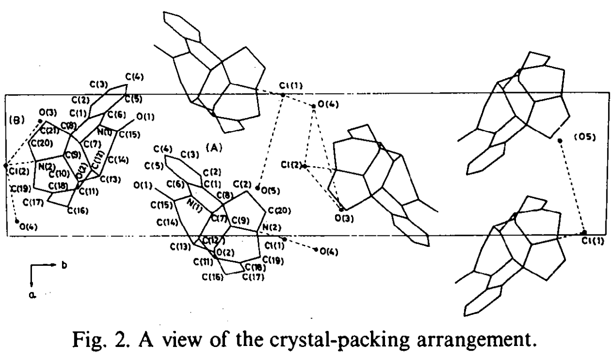

Fig. 2. A view of the crystal-packing arrangement.

The strychnine is protonated at N(2). The values of the bond angles about N(2) are in good agreement with the corresponding values in strychnine sulfonic acid tetrahydrate.

A view of the crystal structure of strychnine hydrochloride along the *c* axis (Fig. 2), reveals the nature of the packing and the hydrogen-bonding arrangement. The structure is stabilized by a three-dimensional network of hydrogen bonds. The N—H···Cl-type hydrogen bonds which contribute to this network are N(2)···Cl(1) [2·987 (5) Å in molecule *A*] and N(2)···Cl(2) [3·064 (5) Å in molecule *B*]. The water molecules between the strychnine molecules are involved in hydrogen bonding of the O—H···Cl and O—H···O types; although one of the H atoms attached to O(3) could not be located, O(3)···Cl(2) [3·181 (6) Å] was assumed to be a hydrogen bond, and others are O(3)···O(4) 2·816 (8), O(4)···Cl(1) 3·129 (6), O(5)···Cl(1) 3·184 (7) Å. The bonds are of complex zigzag configuration. This three-dimensional hydrogen-bond network, which represents the main type of intermolecular interaction, apparently accounts for the somewhat high melting point of the compound.

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Structure and Conformational Analysis of the Opioid Antagonist (−)-(1*R*,5*R*,9*R*)-5,9-Diethyl-2-(3-furylmethyl)-2′-hydroxy-6,7-benzomorphan (Mr2266)*†

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Abstract. $C_{21}H_{27}NO_2$, M_r = 325·449, monoclinic, $P2_1$, a = 16·3916 (7), b = 12·7460 (5), c = 8·9806 (5) Å, β = 107·191 (4)°, V = 1792·5 (2) Å^3, Z = 4, D_m = 1·22 (2), D_x = 1·206 Mg m^{-3}, λ(Cu $K\alpha$) = 1·54178 Å, μ(Cu $K\alpha$) = 0·566 mm^{-1}, $F(000)$ = 704, T = 291 K, final R = 0·048 for 4225 observed reflections. The two molecules present in the asymmetric unit adopt a different conformation with respect to the *N*-side chain. Starting from the asymmetric carbon and proceeding along the allyl moiety the conformations are antiperiplanar/(−)-anticlinal for molecule 1 and antiperiplanar/(+)-synclinal for molecule 2. The furyl rings engage in aromatic–aromatic interactions which are compared with results from a theoretical study from the literature. Finally, the 3-furyl geometry is evaluated through a Cambridge Structural Database search and *CNDO*/2 calculations.

Introduction. In a search for new opioid antagonists within a series of *N*-furylmethyl-substituted 6,7-benzomorphans the title compound was characterized as a pure antagonist about as potent as naloxone (Merz, Langbein, Stockhaus, Walther & Wick, 1974). Depending upon the furyl substitution pattern, the action profile could resemble that of a mixed antagonist(agonist) in the *N*-(2-furylmethyl) derivative, that of a mixed agonist–antagonist in the *N*-(3-methylfurfuryl) derivative, or that of a pure

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* *Chemical Abstracts* name: (−)-(2*R*,6*R*,11*R*)-6,11-diethyl-3-(3-furylmethyl)-1,2,3,4,5,6-hexahydro-2,6-methano-3-benzazocin-8-ol.

† Structural Studies of Substituted 6,7-Benzomorphan Compounds. XV. Part XIV: Verlinde, Blaton, De Ranter & Peeters (1989).

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