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Structures of Lorazepam* Isopropyl Alcohol Solvate (I) and Isoamyl Alcohol Solvate (II)

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Abstract. (I): $C_{15}H_{10}Cl_2N_2O_2.0{\cdot}5C_3H_8O$, $M_r = 351{\cdot}21$, triclinic, $P\bar{1}$, $a = 16{\cdot}563$ (7), $b = 10{\cdot}558$ (3), $c = 10{\cdot}297$ (4) Å, $\alpha = 113{\cdot}20$ (2), $\beta = 90{\cdot}58$ (3), $\gamma = 90{\cdot}98$ (3)°, $V = 1655$ (1) Å^3, $Z = 4$, $D_x = 1{\cdot}41$ g cm^{-3}, $\mu = 4{\cdot}2$ cm^{-1}, λ(Mo $K\alpha$) = 0·71069 Å, $F(000) = 724$, $T = 291$ K, $R = 0{\cdot}050$ for 4679 observed reflections. (II): $C_{15}H_{10}Cl_2N_2O_2.C_5H_{12}O$, $M_r = 409{\cdot}31$, triclinic, $P\bar{1}$, $a = 12{\cdot}923$ (7), $b = 10{\cdot}271$ (5), $c = 8{\cdot}687$ (3) Å, $\alpha = 69{\cdot}91$ (3), $\beta = 72{\cdot}68$ (3), $\gamma = 85{\cdot}33$ (4)°, $V = 1033{\cdot}5$ (8) Å^3, $Z = 2$, $D_x = 1{\cdot}315$ g cm^{-3}, $\mu = 3{\cdot}5$ cm^{-1}, λ(Mo $K\alpha$) = 0·71069 Å, $F(000) = 428$, $T = 291$ K, $R = 0{\cdot}068$ for 2809 observed reflections. In common with several other benzodiazepines the seven-membered ring is in a boat conformation in both molecules (I) and (II). The angle between the benzene ring of the 1,4-benzodiazepine system and the aromatic 5-substituent is 84·6 (5) and 82·6 (5)° for the two independent molecules of (I), and 85·5 (5)° in (II). The two solvates differ in the number of hydrogen bonds between lorazepam and the solvent.

Introduction. Bandoli & Clemente (1976) published the molecular and electronic structure of lorazepam. They found a formulation in which one ethanol molecule is present for two lorazepam molecules. Several structural studies of benzodiazepines have been published since then (Gilli, Bertolasi, Sacerdoti & Borea, 1977, 1978*a*, *b*; Chananont, Hamor & Martin, 1980, 1981; Butcher, Hamor & Martin, 1983; Butcher & Hamor, 1985) but only one of them has shown a solvate molecule (Chananont, Hamor & Martin, 1980). In our study on the polymorphism of lorazepam we have recrystallized the molecule from five solvents (Rambaud, Maury, Pauvert, Delarbre & Lasserre, 1987) and have found five different solvates. In this paper we present the structural study of two of these: the isopropyl alcohol solvate (I) and the isoamyl alcohol solvate (II).

Experimental. (I): obtained by recrystallization from isopropyl alcohol at room temperature, colourless prismatic crystal 0·16 × 0·21 × 0·29 mm. Lattice parameters refined using 15 reflections in the range $5 \le 2\theta \le 25°$. No absorption correction. Syntex $P2_1$ diffractometer, graphite-monochromatized Mo $K\alpha$ radiation. 7608 independent reflections with $(\sin\theta)/\lambda \le 0{\cdot}649$ Å^{-1}, 4679 with $I \ge 2{\cdot}5\sigma(I)$. Index range h −21/21, k−13/12, l 0/13. Standard reflection $(5\bar{1}\bar{2})$ checked every 50 reflections. No significant deviation. Structure solved by direct methods using *SHELX*84 (Sheldrick, 1984). H atoms of lorazepam from difference Fourier synthesis. H atoms of isopropyl alcohol included in the calculation in theoretical positions, their coordinates were not refined. Anisotropic least-squares refinement on F with *SHELX*76 (Sheldrick, 1976). H isotropic with common refined temperature factor ($B_{eq} = 4{\cdot}75$ Å^2). The atoms of isopropyl alcohol, principally C(*S*), show some tendency towards disorder and a difference Fourier synthesis showed a strong peak, with a residual electron density 1·2 e Å^{-3},

* Lorazepam: 7-chloro-5-(2-chlorophenyl)-1,3-dihydro-3-hydroxy-2*H*-1,4-benzodiazepin-2-one.

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Table 1. *Fractional atomic coordinates* ($\times 10^4$) *with e.s.d.'s in parentheses and equivalent isotropic temperature factors* (Å^2) *for non-hydrogen atoms of* (I)

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

	Molecule *A*				Molecule *B*			
	x	*y*	*z*	B_{eq}	*x*	*y*	*z*	B_{eq}
Cl(1)	8124 (1)	7946 (1)	1681 (1)	4·8	9339 (1)	5185 (1)	−3079 (1)	4·9
C(7)	7150 (2)	7563 (3)	954 (3)	3·2	10306 (2)	5450 (3)	−2318 (3)	3·4
C(8)	6513 (2)	7456 (3)	1775 (3)	3·5	10961 (2)	4879 (4)	−3164 (3)	3·7
C(9)	5759 (2)	7128 (3)	1170 (3)	3·3	11717 (2)	5077 (3)	−2554 (3)	3·5
C(10)	5627 (2)	6867 (3)	−257 (3)	2·6	11832 (2)	5825 (3)	−1105 (3)	2·7
C(11)	6261 (2)	7028 (3)	−1062 (3)	2·4	11171 (2)	6435 (3)	−261 (3)	2·5
C(6)	7030 (2)	7390 (3)	−431 (3)	2·8	10402 (2)	6222 (3)	−901 (3)	3·0
N(1)	4833 (1)	6518 (3)	−815 (3)	2·9	12625 (1)	6031 (3)	−569 (3)	3·1
C(2)	4616 (2)	5589 (3)	−2125 (3)	2·5	12880 (2)	6124 (3)	724 (3)	2·6
O(12)	3912 (1)	5329 (2)	−2522 (2)	3·3	13583 (1)	6374 (2)	1112 (2)	3·3
C(3)	5319 (2)	4891 (3)	−3050 (3)	2·3	12218 (2)	5905 (3)	1636 (3)	2·6
O(13)	5075 (1)	3718 (2)	−4213 (2)	2·9	12529 (1)	5627 (2)	2757 (2)	3·2
N(4)	5714 (1)	5907 (2)	−3482 (2)	2·3	11743 (1)	7159 (2)	2144 (2)	2·5
C(5)	6154 (2)	6845 (3)	−2561 (3)	2·3	11274 (2)	7351 (3)	1255 (3)	2·5
C(14)	6620 (2)	7798 (3)	−3046 (3)	2·6	10785 (2)	8628 (3)	1787 (3)	2·9
C(15)	6468 (2)	9191 (3)	−2576 (3)	3·3	10915 (2)	9696 (4)	1323 (4)	4·1
Cl(2)	5720 (1)	9903 (1)	−1336 (1)	6·1	11661 (1)	9536 (1)	104 (1)	5·9
C(16)	6891 (2)	10042 (3)	−3078 (4)	4·3	10485 (3)	10884 (4)	1841 (5)	6·0
C(17)	7499 (2)	9504 (4)	−4028 (4)	4·6	9901 (3)	11038 (5)	2854 (5)	6·7
C(18)	7673 (2)	8150 (4)	−4480 (4)	5·0	9764 (2)	10026 (5)	3327 (4)	5·7
C(19)	7230 (2)	7286 (3)	−4016 (4)	4·1	10206 (2)	8817 (4)	2813 (4)	4·3
Solvent								
C(*S*1)	7763 (3)	2043 (6)	3795 (5)	7·8				
C(*S*2)*	6904 (4)	2433 (9)	3872 (6)	4·5				
C(*S*3)	6392 (4)	1465 (6)	2665 (5)	8·8				
O(*S*)	6593 (1)	2349 (3)	5191 (3)	5·0				
C(*S*2b)	6851 (11)	1580 (36)	3927 (16)	6·3				

* Disordered, see text.

consistent with a second possible position for C(*S*2). The respective site occupation factors are 0·68 C(*S*2) and 0·32 C(*S*2*b*). The values of anisotropic thermal parameters for the isopropyl molecule remain reasonable ($B_{eq} = 4{\cdot}5$ to 8·8 Å^2), $R = 0{\cdot}050$, $wR = 0{\cdot}058$, $S = 1{\cdot}16$ for 4679 observed reflections. Final max. $\Delta/\sigma = 0{\cdot}6$, max. and min. heights in final difference Fourier synthesis 0·58 and −0·42 e Å^{-3}.

(II): obtained by recrystallization in isoamyl alcohol at room temperature, colourless prismatic crystal 0·29 × 0·20 × 0·42 mm. Lattice parameters refined using 15 reflections in the range $3 \le 2\theta \le 17°$. Syntex $P2_1$ diffractometer, graphite-monochromatized Mo $K\alpha$ radiation. No absorption correction. 4753 independent reflections with $(\sin\theta)/\lambda \le 0{\cdot}649$ Å^{-1}, 2809 with $I \ge 2{\cdot}5\sigma(I)$. Index range $h -16/16$, $k -12/13$, $l 0/11$. Standard reflection $(4\bar{2}1)$ checked every 50 reflections. No significant deviation. Structure solved by direct methods using *SHELX*84 (Sheldrick, 1984). H atoms of lorazepam from difference Fourier synthesis. Anisotropic least-squares refinement on F with *SHELX*76 (Sheldrick, 1976). H isotropic with common refined temperature factor ($B_{eq} = 4{\cdot}74$ Å^2). The atoms of the isoamyl alcohol showed some tendency towards disorder after four cycles of anisotropic refinement; the difference Fourier synthesis at $R = 0{\cdot}09$ gave the two strongest peaks with residual electron density 1·6 and 1·2 e Å^{-3}. The peaks were identified as C(*S*2*b*) and C(*S*2*c*) and were included in further cycles. The respective site occupation factors are 0·60 C(*S*2), 0·20 C(*S*2*b*) and 0·20 C(*S*2*c*). H atoms at C(*S*4) and C(*S*5) were included in the calculation in theoretical positions and their coordinates were not refined. Four cycles of refinement give $R = 0{\cdot}068$, $wR = 0{\cdot}074$, $S = 2{\cdot}43$ for 2809 observed reflections, $w = 1/[\sigma^2(F) + 0{\cdot}00047\,F^2]$. Final max. $\Delta/\sigma = 0{\cdot}8$, max. and min. heights in final difference Fourier synthesis 0·38 and −0·47 e Å^{-3}.

Atomic scattering factors from *International Tables for X-ray Crystallography* (1974).

Discussion. Final atomic coordinates are given in Tables 1 and 2.* Table 3 gives the comparative values of bond distances. The structures are shown in Fig. 1.

Bond lengths and angles agree well with values found in lorazepam ethanol solvate (Bandoli & Clemente, 1976). By comparison with other analogous molecules, the ring angle at N(1) is in good agreement with that in N(1)—H benzodiazepines (Chananont *et al.*, 1981; Gilli

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters and valence angles for (I) and (II) have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44089 (39 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Fractional atomic coordinates* ($\times 10^4$) *with e.s.d.'s in parentheses and equivalent isotropic temperature factors* (Å^2) *for non-hydrogen atoms of* (II)

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

	x	y	z	B_{eq}
Cl(1)	2277 (1)	6839 (1)	4423 (2)	5·60
Cl(2)	3612 (1)	2020 (2)	1939 (2)	8·75
N(1)	508 (3)	1851 (4)	4073 (4)	3·76
N(4)	1150 (3)	3430 (3)	336 (4)	3·32
O(12)	−303 (3)	664 (3)	2970 (3)	4·74
O(13)	−662 (3)	3051 (3)	520 (4)	4·58
C(7)	1798 (3)	5359 (4)	4294 (5)	3·89
C(8)	1232 (4)	4340 (4)	5796 (5)	4·11
C(9)	804 (4)	3216 (5)	5675 (5)	3·98
C(10)	939 (3)	3056 (4)	4090 (4)	3·30
C(11)	1556 (3)	4050 (4)	2598 (4)	3·22
C(6)	1971 (3)	5204 (4)	2731 (5)	3·66
C(2)	58 (3)	1765 (4)	2893 (5)	3·71
C(3)	38 (3)	3126 (4)	1438 (5)	3·49
C(5)	1814 (3)	3870 (4)	897 (4)	3·19
C(14)	2941 (3)	4239 (4)	−258 (5)	3·61
C(15)	3823 (4)	3468 (5)	97 (6)	5·04
C(16)	4858 (4)	3766 (7)	−1006 (8)	6·64
C(17)	5016 (5)	4882 (7)	−2488 (8)	6·72
C(18)	4157 (5)	5674 (6)	−2882 (7)	6·16
C(19)	3137 (4)	5356 (5)	−1781 (5)	4·71
O(5)	889 (3)	−810 (4)	559 (5)	6·99
C(*S*1)	1890 (6)	−397 (10)	536 (10)	11·04
C(*S*2)*	2834 (8)	−713 (12)	−772 (13)	8·36
C(*S*3)	2872 (11)	393 (13)	−2492 (13)	14·31
C(*S*4)	3378 (10)	−459 (12)	−3424 (16)	18·42
C(*S*5)	3518 (8)	1720 (11)	−3272 (13)	13·16
C(*S*2*b*)*	2676 (24)	382 (29)	−655 (34)	5·61
C(*S*2*c*)*	2021 (27)	445 (32)	−1162 (43)	7·00

* Disordered, see text.

Table 3. *Bond distances* (Å) *with e.s.d.'s in parentheses*

	(I)		
	(*A*)	(*B*)	(II)
C(7)–Cl(1)	1·744 (3)	1·745 (3)	1·736 (4)
C(8)–C(7)	1·390 (5)	1·388 (4)	1·398 (6)
C(6)–C(7)	1·376 (5)	1·360 (4)	1·371 (5)
C(9)–C(8)	1·367 (5)	1·370 (5)	1·367 (6)
C(10)–C(9)	1·399 (4)	1·395 (4)	1·400 (5)
C(11)–C(10)	1·393 (4)	1·405 (4)	1·402 (5)
N(1)–C(10)	1·413 (4)	1·399 (4)	1·405 (5)
C(2)–N(1)	1·358 (3)	1·359 (4)	1·350 (5)
O(12)–C(2)	1·222 (3)	1·217 (3)	1·231 (4)
C(3)–C(2)	1·519 (4)	1·524 (4)	1·534 (5)
O(13)–C(3)	1·392 (3)	1·394 (4)	1·394 (5)
N(4)–C(3)	1·461 (4)	1·464 (4)	1·459 (5)
C(5)–N(4)	1·278 (3)	1·273 (4)	1·282 (5)
C(6)–C(11)	1·400 (4)	1·401 (4)	1·393 (5)
C(5)–C(11)	1·487 (4)	1·483 (3)	1·488 (5)
C(14)–C(5)	1·494 (4)	1·496 (4)	1·492 (5)
C(15)–C(14)	1·384 (4)	1·401 (5)	1·384 (6)
C(19)–C(14)	1·387 (4)	1·390 (5)	1·391 (6)
Cl(2)–C(15)	1·742 (3)	1·732 (4)	1·738 (5)
C(16)–C(15)	1·384 (6)	1·370 (5)	1·380 (7)
C(17)–C(16)	1·376 (5)	1·393 (5)	1·370 (8)
C(18)–C(17)	1·355 (5)	1·355 (8)	1·378 (8)
C(19)–C(18)	1·388 (6)	1·397 (6)	1·366 (7)
Isoamyl alcohol		Isopropyl alcohol	
C(*S*1)–O(*S*)	1·387 (8)	C(*S*1)–C(S2)	1·482 (8)
C(*S*2)–C(*S*1)	1·499 (1)	C(*S*3)–C(S2)	1·501 (8)
C(*S*3)–C(*S*2)	1·525 (14)	C(*S*2)–O(S)	1·492 (8)
C(*S*4)–C(*S*3)	1·388 (12)		
C(*S*5)–C(*S*3)	1·493 (13)		

et al., 1977, 1978*a*; Butcher *et al.*, 1983) but differs from that in N(1)–Me substituted benzodiazepines (Chananont *et al.*, 1981; Butcher *et al.*, 1983; Butcher & Hamor, 1985; Gilli *et al.*, 1978*b*). Similar differences have been noted previously by Chananont *et al.* (1981) and Butcher *et al.* (1983). We also found some differences around C(3): it appears that substitution of C(3)–H by hydroxyl causes an increase in the C(2)–C(3)–N(4) angle by some 2–3°.

In common with other benzodiazepines, the seven-membered ring adopts a boat conformation with C(3) at the bow and C(10)–C(11) at the stern. If we take N(1)–C(2)–N(4)–C(5) as base plane, least-squares-planes calculations give a 'bow angle' of 61·2 (5)° for (II) and 61·9 (5) and 62·0 (5)° for the two independent molecules of (I). The stern angles are 32·8 (5)° for (II) and 32·5 (5) and 31·6 (5)° for (I). These values are the same as those found in the ethanol solvate (Bandoli & Clemente, 1976).

The major conformational difference between the title compounds and other benzodiazepines is in the orientation of the 5-phenyl ring to the benzene ring of the benzodiazepine. However, the values of 88·9 (5)° in (II) and 88·4 (5) and 84·9 (5)° in (I) (*XANADU:* Roberts & Sheldrick, 1975) agree well with the values given by Chananont *et al.* (1981) for the benzodiazepine where the 5-phenyl ring also carries an *o*-chloro substituent.

Intermolecular contact distances are listed in Table 4. In the three lorazepam solvates, *i.e.* ethanol solvate

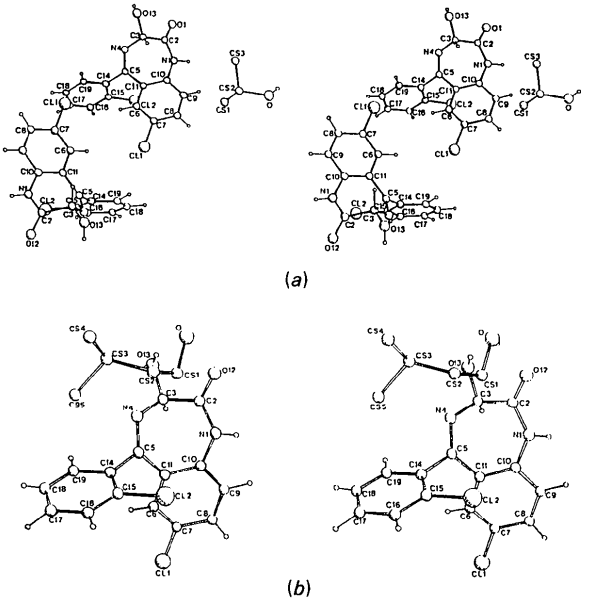

Fig. 1. Stereoscopic views of (*a*) lorazepam isopropyl alcohol solvate, (I) and (*b*) lorazepam isoamyl alcohol solvate, (II), drawn with *PLUTO*78 (Motherwell & Clegg, 1978).

Table 4. *Hydrogen bonds* (Å)

Structure (I) (e.s.d.'s are *ca* 0·004 Å)

N(1')···O(12^{i})	2·846 Å
N(1)···O(12^{ii})	2·925
O(13)···N(4^{iii})	2·862
O(13')···O(S^{iv})	2·724
O(S)···O(13^{v})	2·872

Symmetry codes: (i) $1+x, y, z$; (ii) $x-1, y, z$; (iii) $1-x, 1-y, -1-z$; (iv) $2-x, 1-y, 1-z$; (v) $x, y, 1+z$.

Structure (II) (e.s.d.'s are *ca* 0·005 Å)

N(1)···O(12^{i})	2·931
O(13)···O(S^{ii})	2·823
O(S)···O(S^{iii})	2·936
O(S)···O(12)	2·985

Symmetry codes: (i) $-x, -y, 1-z$; (ii) x, y, z.

(Bandoli & Clemente 1976), isopropyl alcohol solvate and isoamyl alcohol solvate, the solvent is efficient in the cohesion of the crystal. In (II) the number of hydrogen bonds between lorazepam and the solvent is greater than in the other two solvates. For all three solvates the intermolecular hydrogen bonding between N(1)—H of the reference molecule (x, y, z) and the C(2)—O(12) keto group of the molecule at ($-x, -y, -z$) for ethanol solvate, ($-x, -y, 1-z$) for (II) and ($1+x, y, z$) for (I) forms lorazepam dimers *via* a ring of eight atoms. It is interesting to note that this benzodiazepine exhibits, in addition to its capacity to form solvates, a number of hydrogen bonds more important than those found in other analogues.

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The Structure of an Aziridine Derivative

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Abstract. 1,2-Bis(dimethylaminosulfonyl)-1,1a,1b,-2-tetrahydroaziridino[1,2-*a*]cyclopropano[*c*]naphthyridene, $C_{14}H_{20}N_4O_4S_2$, $M_r = 372{\cdot}5$, triclinic, $P\bar{1}$, $a = 9{\cdot}171$ (2), $b = 9{\cdot}918$ (2), $c = 10{\cdot}699$ (2) Å, $\alpha = 84{\cdot}86$ (2), $\beta = 79{\cdot}57$ (1), $\gamma = 62{\cdot}28$ (2)°, $V = 847{\cdot}2$ Å^3, $Z = 2$, $D_m = 1{\cdot}45$, $D_x = 1{\cdot}460$ g cm^{-3}, Cu $K\alpha$, $\lambda = 1{\cdot}54178$ Å, $\mu = 29{\cdot}51$ cm^{-1}, $F(000) = 392$, $T = 293$ K, $R = 0{\cdot}0531$, $wR = 0{\cdot}0561$ for 3100 observed reflections. The central part of the molecule is nearly planar with the cyclopropane and aziridine rings bent in opposite directions. The cyclopropane and aziridine rings make dihedral angles of 108·2 and 75·7° respectively with the naphthyridine plane.

Introduction. This investigation is the second in a series of structure determinations of bis(aziridine) and cyclopropaneaziridine derivatives obtained in the reaction of

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