

N(7)	0,5431 (3)	0,2011 (1)	0,0563 (2)	3,42 (5)
C(8)	0,5050 (3)	0,2440 (2)	-0,0595 (3)	3,30 (6)
C(9)	0,4525 (3)	0,3166 (1)	-0,0284 (3)	3,56 (6)
C(10)	0,2725 (3)	0,3219 (1)	-0,0555 (3)	3,71 (7)
C(11)	0,1977 (3)	0,3258 (2)	0,0602 (3)	4,08 (7)
C(12)	0,0333 (4)	0,3313 (2)	0,0333 (4)	5,07 (8)
C(13)	-0,0592 (4)	0,3325 (2)	-0,1066 (4)	6,4 (1)
C(14)	0,0151 (4)	0,3296 (2)	-0,2221 (4)	6,7 (1)
C(15)	0,1813 (4)	0,3241 (2)	-0,1990 (4)	5,31 (9)
C(16)	0,7914 (5)	-0,0001 (2)	-0,1459 (5)	8,0 (1)
C(17)	0,6533 (6)	0,0029 (2)	0,3526 (4)	8,7 (1)
O(18)	0,5100 (2)	0,2261 (1)	-0,1849 (2)	4,74 (5)
N(19)	-0,0431 (3)	0,3379 (2)	0,1580 (4)	6,82 (8)
O(20)	0,0402 (3)	0,3472 (2)	0,2796 (3)	7,97 (7)
O(21)	-0,1877 (3)	0,3339 (2)	0,1350 (3)	11,0 (1)

Tableau 2. Longueurs (Å), angles des liaisons (°) et écarts-type

N(1)—C(2)	1,333 (4)	C(8)—O(18)	1,231 (3)
N(1)—C(6)	1,342 (4)	C(9)—C(10)	1,515 (4)
C(2)—C(3)	1,375 (4)	C(10)—C(11)	1,375 (5)
C(2)—N(7)	1,416 (4)	C(10)—C(15)	1,399 (4)
C(3)—C(4)	1,391 (4)	C(11)—C(12)	1,384 (4)
C(4)—C(5)	1,377 (5)	C(12)—C(13)	1,375 (5)
C(4)—C(16)	1,512 (6)	C(12)—N(19)	1,461 (5)
C(5)—C(6)	1,374 (5)	C(13)—C(14)	1,369 (6)
C(6)—C(17)	1,510 (5)	C(14)—C(15)	1,401 (5)
N(7)—C(8)	1,341 (3)	N(19)—O(20)	1,217 (4)
C(8)—C(9)	1,511 (4)	N(19)—O(21)	1,217 (4)
C(2)—N(1)—C(6)	117,1 (3)	C(9)—C(8)—O(18)	120,9 (2)
N(1)—C(2)—C(3)	124,4 (3)	C(8)—C(9)—C(10)	111,5 (2)
N(1)—C(2)—N(7)	111,6 (2)	C(9)—C(10)—C(11)	120,4 (2)
C(3)—C(2)—N(7)	123,9 (3)	C(9)—C(10)—C(15)	120,1 (3)
C(2)—C(3)—C(4)	117,8 (3)	C(11)—C(10)—C(15)	119,4 (3)
C(3)—C(4)—C(5)	118,5 (3)	C(10)—C(11)—C(12)	119,6 (3)
C(3)—C(4)—C(16)	119,8 (3)	C(11)—C(12)—C(13)	122,1 (3)
C(5)—C(4)—C(16)	121,7 (3)	C(11)—C(12)—N(19)	118,6 (3)
C(4)—C(5)—C(16)	119,7 (3)	C(13)—C(12)—N(19)	119,3 (3)
N(1)—C(6)—C(5)	122,6 (3)	C(12)—C(13)—C(14)	118,4 (3)
N(1)—C(6)—C(17)	115,2 (3)	C(13)—C(14)—C(15)	121,1 (3)
C(5)—C(6)—C(17)	122,2 (3)	C(10)—C(15)—C(14)	119,4 (3)
C(2)—N(7)—C(8)	128,3 (2)	C(12)—N(19)—O(20)	118,8 (3)
N(7)—C(8)—C(9)	116,2 (2)	C(12)—N(19)—O(21)	118,2 (3)
N(7)—C(8)—O(18)	122,9 (3)	O(20)—N(19)—O(21)	123,0 (3)

La solution trouvée initialement en utilisant le programme *MULTAN11/82* (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982) comportait une erreur d'origine. Pour cette raison, la structure a été résolue en admettant pour groupe spatial le groupe *Pc*. Une origine compatible avec les éléments de symétrie du groupe *P2₁/c* a ensuite été déduite des positions atomiques ainsi obtenues.

Les calculs ont été effectués avec les programmes du système *SDP* (B. A. Frenz & Associates, Inc., 1982) et les Fig. 1 et 2 réalisées avec le programme *ORTEPII* (Johnson, 1976). Les coordonnées atomiques relatives sont rapportées dans le Tableau 1, les longueurs et les angles des liaisons dans le Tableau 2. La Fig. 1 représente la molécule et indique les numéros attribués à ses atomes et la Fig. 2 une vue de la structure.

Les listes des facteurs de structure, des facteurs d'agitation thermique anisotrope, des coordonnées des atomes d'hydrogène, des distances C—H et N—H, des distances interatomiques intermoléculaires des distances des atomes aux plans moyens, et des angles de torsion ont été déposées au dépôt d'archives de la British Library Document Supply Centre (Supplementary Publication No. SUP 55440: 14 pp.). On peut en obtenir des copies en s'adressant à: The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, Angleterre. [Référence de CIF: PA1009]

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2,4-Dimethyl-(1*H*)-naphtho[2,3-*b*]-[1,5]diazepinium Chloride Monohydrate

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Abstract

The cation derived from the title compound is planar. All the atoms in the seven-membered ring are *sp*² hybridized and the electrons are delocalized over the ring. The molecules are stacked in parallel sheets and linked to chloride ions and water molecules by hydrogen bonding. Chloride ions and water molecules are arranged in square-planar units which are approximately perpendicular to the plane of the aromatic rings. Charge distributions for the title compound were calculated from crystallographic data by the *AM1* semi-empirical method and compared with those for 2,2,4-trimethyl-2,3-dihydro-

(1*H*)-1,5-benzodiazepine chloride. Calculations show that, in both compounds, the entire positive charge is not localized on the N atoms but delocalized over the neighbouring atoms.

Comment

A great number of diazepine analogs are used as anxiolytic, sedative-hypnotic or anticonvulsant drugs. Some of these, mainly 2,4-disubstituted compounds, have interesting chromogenic properties which are used for analytical purposes.

The title compound (I) was synthesized using β -diketones and characterized by NMR and IR methods. However, these methods did not determine a definite structure. It is known that the seven-membered ring of the benzodiazepine derivatives possesses great flexibility which is dependent on the variation of pH (Suresh, Prabhakar & Kulkarni, 1988). In order to ascertain the geometry of this molecule unequivocally, the chloride was crystallized from methanol solution for crystallographic study.

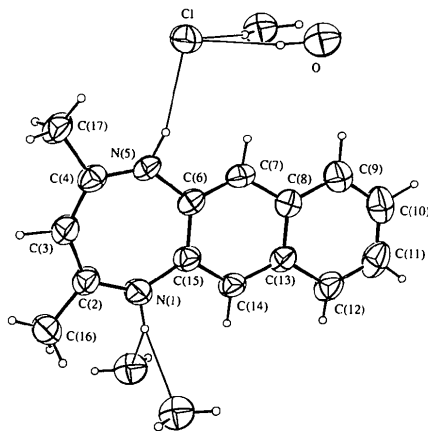


Fig. 1. The title molecule with atom numbering.

Bond lengths and angles in (I) are similar to those observed in related compounds. The values of torsion angles are near to 0 and 180° [-2.6 (5)– 1.7 (5)° and -179.5 (3)– 180.0 (3)°]. The molecule is planar, with the exception of the H atoms of the methyl groups. All the atoms in the seven-membered ring are sp^2 hybridized and the electrons are delocalized over the whole ring. In contrast to the closely related 2,2,4-trimethyl-2,3-dihydro-(1*H*)-1,5-benzodiazepine hydrochloride (II) (Abramenko, Sergienko, Garnovskii & Porai-Kochitz, 1990), the seven-membered ring is not planar and there is no electron delocalization. The molecules are stacked in parallel sheets and linked to chloride ions and water molecules by hydrogen interactions. Chloride ions and water molecules are arranged in square-planar units which are approximately perpendicular to the planes of the aromatic rings (Fig. 2).

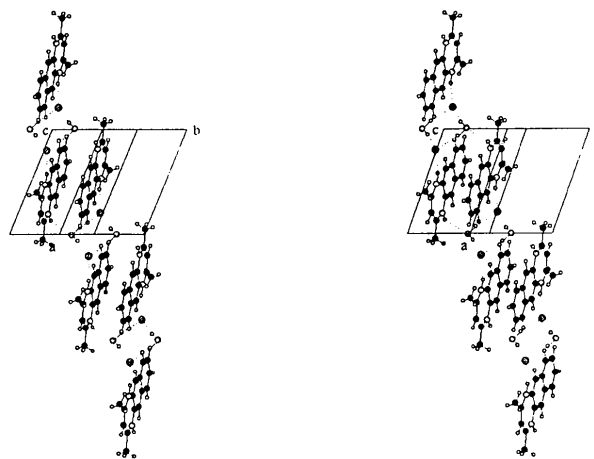


Fig. 2. Stereoview of the lattice with unit cell. Dotted lines represent hydrogen bonds.

It has been proposed that one important element of a drug–receptor interaction may be an ionic or electrostatic bond located at an anionic site on the receptor surface (Beckett, 1956). The activity of the same nitrogen-containing compounds has been related to charge distribution within the molecule (Frimowitz, Neumeyer & Baldessarini, 1986). We therefore performed semi-empirical charge calculations on (I) and, for comparison, (II) using the *AM1* Hamiltonian (Dewar, Zoebisch, Healy & Stewart, 1985).

AM1 charge variation shows clearly that for the cation, the +1 charge is not localized on the N atom which has just been protonated as was supposed for (II) (Abramenko *et al.*, 1990) but distributed over several atoms. For (II), the charge variation is confined to the same N atom and the adjacent C atom in the seven-membered ring. For (I), owing to conjugation, the charge is also spread over the other unprotonated N atom and the C atom α to this atom (Fig. 3). Similar observations have already been

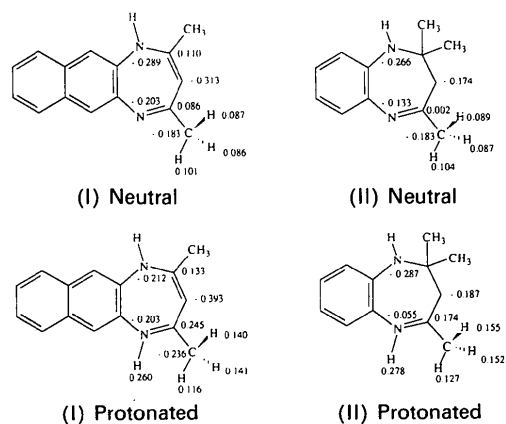


Fig. 3. Selected *AM1* charges for neutral and protonated (I) and (II).

published for charges calculated by the *CNDO/2* semi-empirical method on morphine analogs (Saethre, Carlson, Kaufman & Koski, 1975).

For the methyl groups situated in an α position with respect to the protonated N atom, the charge increase is higher for the two H atoms out of the plane of the seven-membered ring than for the H atom located in the plane of the ring. This may be explained by hyperconjugation, *i.e.* the overlap of the σ orbital of the C—H bond and the π orbital of the C=N bond (March, 1985).

C(3)	0.8044 (3)	0.4656 (5)	0.3334 (3)	4.37 (8)
C(4)	0.6503 (3)	0.3840 (4)	0.3155 (3)	3.71 (7)
N(5)	0.5324 (2)	0.3063 (4)	0.2056 (2)	3.79 (6)
C(6)	0.5258 (3)	0.2779 (4)	0.0768 (2)	3.30 (7)
C(7)	0.3823 (3)	0.1867 (4)	-0.0129 (3)	3.52 (7)
C(8)	0.3539 (3)	0.1483 (4)	-0.1472 (3)	3.48 (7)
C(9)	0.2051 (3)	0.0536 (5)	-0.2399 (3)	4.55 (9)
C(10)	0.1865 (4)	0.0254 (5)	-0.3654 (3)	5.2 (1)
C(11)	0.3137 (4)	0.0923 (5)	-0.4035 (3)	5.3 (1)
C(12)	0.4593 (3)	0.1834 (5)	-0.3150 (3)	4.61 (9)
C(13)	0.4829 (3)	0.2129 (4)	-0.1837 (3)	3.45 (7)
C(14)	0.6310 (3)	0.3061 (5)	-0.0878 (3)	3.64 (7)
C(15)	0.6540 (3)	0.3390 (4)	0.0385 (2)	3.41 (7)
C(16)	1.0490 (3)	0.5909 (6)	0.2946 (3)	5.4 (1)
C(17)	0.6060 (3)	0.3786 (5)	0.4306 (3)	4.96 (9)
O	-0.0020 (2)	0.2684 (3)	0.0048 (2)	5.35 (6)

Experimental

Crystal data

$C_{15}H_{15}N_2^+Cl^- \cdot H_2O$

$M_r = 276.78$

Triclinic

$P\bar{1}$

$a = 10.276 (1) \text{ \AA}$

$b = 7.091 (1) \text{ \AA}$

$c = 11.3800 (9) \text{ \AA}$

$\alpha = 98.79 (1)^\circ$

$\beta = 105.26 (1)^\circ$

$\gamma = 115.23 (1)^\circ$

$V = 689.5 (4) \text{ \AA}^3$

$Z = 2$

$D_x = 1.338 \text{ Mg m}^{-3}$

Data collection

Enraf-Nonius CAD-4

diffractometer

$\theta/2\theta$ scans

Absorption correction:

none

1926 measured reflections

1926 independent reflections

1399 observed reflections

$[I \geq 3\sigma(I)]$

Refinement

Refinement on F^2

Final $R = 0.041$

$wR = 0.052$

$S = 1.75$

1399 reflections

224 parameters

Only coordinates of H atoms

refined

$w = 1/\sigma^2(F)$

$(\Delta/\sigma)_{\max} = 0.01$

Cu $K\alpha$ radiation

$\lambda = 1.5418 \text{ \AA}$

Cell parameters from 25

reflections

$\theta = 11.44\text{--}28.61^\circ$

$\mu = 2.416 \text{ mm}^{-1}$

$T = 294 \text{ K}$

Approximate parallelepiped

$0.24 \times 0.13 \times 0.05 \text{ mm}$

Black

Crystal source: crystalliza-

tion from methanol solu-

tion

$\theta_{\max} = 58^\circ$

$h = -11 \rightarrow 11$

$k = 0 \rightarrow 7$

$l = -12 \rightarrow 12$

3 standard reflections

frequency: 120 min

intensity variation: 10.8%

intensity variation: 10.8%

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Table 2. Geometric parameters (\AA , $^\circ$)

N(1)—C(2)	1.319 (3)	C(8)—C(13)	1.403 (4)
N(1)—C(15)	1.426 (3)	C(9)—C(10)	1.362 (5)
C(2)—C(3)	1.379 (5)	C(10)—C(11)	1.398 (6)
C(2)—C(16)	1.485 (4)	C(11)—C(12)	1.361 (4)
C(3)—C(4)	1.378 (4)	C(12)—C(13)	1.416 (4)
C(4)—N(5)	1.326 (3)	C(13)—C(14)	1.411 (3)
C(4)—C(17)	1.496 (5)	C(14)—C(15)	1.360 (4)
N(5)—C(6)	1.428 (4)	N(1)···O ⁱ	3.112 (4)
C(6)—C(7)	1.352 (3)	N(1)···O ⁱⁱ	3.028 (4)
C(6)—C(15)	1.409 (4)	N(5)···Cl	3.233 (3)
C(7)—C(8)	1.437 (4)	O···Cl	3.246 (3)
C(8)—C(9)	1.401 (4)	O···Cl ⁱⁱⁱ	3.187 (2)
C(2)—N(1)—C(15)	132.2 (3)	C(8)—C(9)—C(10)	119.6 (3)
N(1)—C(2)—C(3)	126.5 (3)	C(9)—C(10)—C(11)	121.1 (3)
N(1)—C(2)—C(16)	114.4 (3)	C(10)—C(11)—C(12)	120.2 (3)
C(3)—C(2)—C(16)	119.1 (2)	C(11)—C(12)—C(13)	120.2 (3)
C(2)—C(3)—C(4)	130.9 (3)	C(8)—C(13)—C(12)	118.7 (2)
C(3)—C(4)—N(5)	127.3 (3)	C(8)—C(13)—C(14)	118.6 (3)
C(3)—C(4)—C(17)	118.2 (2)	C(12)—C(13)—C(14)	122.7 (3)
N(5)—C(4)—C(17)	114.5 (2)	C(13)—C(14)—C(15)	122.7 (3)
C(4)—N(5)—C(6)	131.5 (3)	N(1)—C(15)—C(6)	125.8 (2)
N(5)—C(6)—C(7)	115.1 (3)	N(1)—C(15)—C(14)	114.9 (3)
N(5)—C(6)—C(15)	125.6 (2)	C(6)—C(15)—C(14)	119.4 (2)
C(7)—C(6)—C(15)	119.3 (3)	N(1)—H(1)···O ⁱ	129 (3)
C(6)—C(7)—C(8)	122.7 (3)	N(1)—H(1)···O ⁱⁱ	142 (4)
C(7)—C(8)—C(9)	122.5 (3)	N(5)—H(5)···Cl	166 (3)
C(7)—C(8)—C(13)	117.3 (2)	O—H(O)···Cl ⁱⁱⁱ	168 (4)
C(9)—C(8)—C(13)	120.1 (3)	O—H'(O)···Cl	170 (3)

Symmetry code: (i) $1 + x, y, z$; (ii) $1 - x, 1 - y, -z$; (iii) $-x, -y, -z$.

The decrease of intensity was corrected for. All calculations were performed using the *SDP* system (B. A. Frenz & Associates, Inc., 1982) using a VAX 3100. The structure was solved by direct methods with *MULTAN* (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982). The molecular structure drawing was prepared using *ORTEPII* (Johnson, 1976). A stereoview of the molecules in the unit cell was obtained with *MOL-DRAW* (Cense, 1989). The *AM1* calculations were performed on a Silicon Graphics 4D/25 using *MOPAC 4.00* (Stewart, 1983). Geometries were fully optimized employing the keyword *PRE-CISE* and without applying any constraints.

Lists of structure factors, anisotropic thermal parameters, H-atom coordinates, bond distances involving H atoms and least-squares-planes data have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55439 (13 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: PA1013]

Table 1. Fractional atomic coordinates and equivalent isotropic thermal parameters (\AA^2)

$$B_{\text{eq}} = (4/3)[\beta_{11}a^2 + \beta_{22}b^2 + \beta_{33}c^2 + (ab \cos \gamma)\beta_{12} + (ac \cos \beta)\beta_{13} + (bc \cos \alpha)\beta_{23}].$$

	x	y	z	B_{eq}
Cl	0.20062 (8)	0.1674 (2)	0.23200 (7)	5.45 (2)
N(1)	0.8116 (3)	0.4375 (4)	0.1217 (2)	4.79 (7)
C(2)	0.8780 (3)	0.4915 (5)	0.2469 (3)	3.92 (8)

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Désoxy-1 *N,N*-Diméthylthiocarbamoyl-1 Di-*O*-isopropylidène-2,3:4,5 Xylitol

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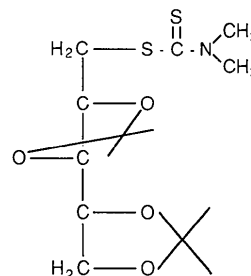
Abstract

The *N,N*-dimethylthiocarbamoyl group is planar. The C(1)O(2)C(3)C(4)O(5) and C(6)O(7)C(8)O(9)-

C(10) five-membered rings adopt envelope and half-chair conformations, respectively. There is a delocalized orbital over the thioamide group. The absolute configuration of the molecule was determined using the anomalous scattering of the two S atoms. Bond lengths and angles are in agreement with published values for similar compounds.

Commentaire

Le produit étudié appartient à une famille d'esters formés par l'acide dithiocarbamique avec des composés d'origine naturelle tels que des polyols et des dérivés monosaccharidiques. La perspective de ce travail est l'obtention de composés qui conservent les propriétés thérapeutiques des dithiocarbamates alcalins mais qui soient plus stables que ces derniers dans les milieux biologiques. Le but de l'étude cristallographique est de préciser la géométrie de la molécule et de déterminer sa configuration absolue.



La valeur de l'angle de torsion endocyclique autour de la liaison C(1)—O(5) [$-0,5$ (4) $^\circ$] indique que C(1), O(2), C(4) et O(5) sont coplanaires. C(3) est situé à 0,538 (4) Å du plan moyen $P(A)$ défini par ces quatre atomes. Le cycle C(1)O(2)C(3)C(4)O(5) possède donc la forme enveloppe. La symétrie dominante (Duax & Norton, 1975) est la symétrie par rapport à un plan passant par C(3) et par le milieu de C(1)—O(5). L'écart à la symétrie idéale s'exprime par la relation $\Delta C_s = 0,8^\circ$.

Le cycle C(6)O(7)C(8)O(9)C(10) a la forme demi-chaise. En effet, O(9) et C(10) sont situés de part et d'autre du plan C(6)C(7)C(8) [plan $P(B)$], le premier à 0,237 (3), le second à 0,291 (4) Å. Il en résulte que la symétrie dominante est la symétrie par rapport à un axe binaire passant par O(7) et par le milieu de O(9)—C(10). Le paramètre d'asymétrie ΔC_2^{9-10} est égal à 1,1 $^\circ$.

Le groupement *N,N*-diméthylthiocarbamate est très proche de la planéité ($\chi^2 = 140$). La distance de C(11) à son plan moyen $P(C)$ est de 0,277 (4) Å. Les angles dièdres $P(A)P(B)$, $P(A)P(C)$ et $P(B)P(C)$ mesurent respectivement 74,0 (2), 52,5 (2) et 59,6 (2) $^\circ$.

Les longueurs des liaisons C—O appartiennent à l'intervalle 1,418 (5)–1,436 (5) Å et admettent pour