by the dihedral angle of 7·6 (2)° between the two rings and the C3—C31 bond length [1·472 (8) Å]; corresponding values for (3) are 35·9 (2)° and 1·467 (6) Å, indicating less conjugation. All the C—N and the N—N bond distances in the heterocyclic rings are intermediate between the expected single- and double-bond lengths. The sums of the valency angles around N1 and N4 in (1) and (3) are 359·3 and 359·6° respectively, indicating no significant pyramidalization of these atoms. From the above results, it is suggested that the triazole rings have aromatic character and the hybridization of the exocyclic nitrogen atom is of the sp^2 type. As in previous reports (Branch & Nowell, 1985, 1986), the exocyclic angles around the N1 atom in compound (1) show considerable asymmetry: C21—N1—C5 [130·0 (5)°] being much larger than C21—N1—N2 [119·4 (5)°]; this asymmetry is also usual in 1,2,3-triazoles (Nagawa, Goto, Honda & Nakanishi, 1987). In molecules (1) and (3), bond angles around C3 are essentially symmetrical, but at C5 there is also a pronounced asymmetry: in (1), N4—C5—C51 and C51—C5—N1 are 128·5 (5) and 122·1 (6)° respectively, while in (3) they are 123·7 (4) and 127·4 (4)° respectively. The benzoyl oxime group is linked to N1 in (1) and to N4 in (3), of the triazole ring. Steric requirements lead the oxime group to be oriented nearly perpendicularly with respect to the heterocyclic ring, as can be seen from the torsion angles C5—N1—C21—N3 [−81·5 (7)°] for (1) and C5—N4—C21—N3 [86·6 (6)°] for (3). C21—N3 bond distances are 1·282 (7) and 1·277 (5) Å, while N3—O1 bond distances are 1·398 (6) and 1·384 (6) Å for (1) and (3) respectively. These values are in the range 1·22 to 1·33 Å for the C—N and 1·357 to 1·439 Å for the N—O bonds (Diànez, Vega, Lòpez-Castro & Màrquez, 1986, and references therein). The oxime configuration in both isomers is *Z*. The benzene ring linked to C21 at 1·476 (8) and 1·477 (8) Å makes angles of 159·3 (5)° and 3·6 (4)° with respect to the C=N—OH fragments of (1) and (3) respectively. This indicates that in (3) there is conjugation over the system.

There are several C···C, C···N, C···C and O···N inter- and intramolecular contacts less than the sums of the van der Waals radii. Some of these, involving the O atom of the oxime group, can be properly described as hydrogen bonds.

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The Structure of 10,11-Dihydro-10-hydroxy-5*H*-dibenz[*b*,*f*]azepine-5-carboxamide, an Anticonvulsant Drug Molecule

By John N. Lisgarten, Rex A. Palmer* and Jose W. Saldanha

Department of Crystallography, Birkbeck College, University of London, Malet Street, London WC1E 7HX, England

(*Received* 29 *June* 1988; *accepted* 4 *November* 1988)

Abstract. $C_{15}H_{14}N_2O_2$, $M_r = 253·40$, orthorhombic, *Pbca*, $a = 7·891$ (5), $b = 13·649$ (8), $c = 23·534$ (4) Å, $V = 2534·7$ (1) Å^3, $Z = 8$, $D_m = 1·33$, $D_x = 1·33$ g cm^{-3}, λ(Cu $K\alpha$) = 1·54184 Å, $\mu = 5·93$ cm^{-1}, $F(000) = 1064$, $T = 293$ K, $R = 0·038$ for 1058 observed reflections. The central azepine ring exists in a twist-boat conformation. Intermolecular hydrogen bonds are formed involving the amide N and hydroxyl O atoms [N···O = 2·916 (7) Å, N—H···O = 161 (5)°], and between the hydroxyl and carbonyl O atoms [O···O = 2·675 (7) Å, O—H···O = 166 (5)°].

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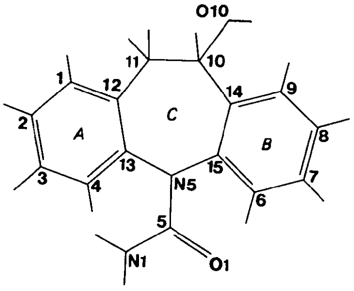
* Author for correspondence.

0108-2701/89/040656-03$03.00

Introduction. The title compound, GPZ (I), is one of a series of iminostilbene derivatives developed as anti-epileptic agents and has proved to be effective as such (Baltzer & Schmutz, 1978). Modification of substituents on C(10) and C(11) of the azepine ring is known to alter anticonvulsant activity significantly (Gagneux, 1976). The structure analysis reported here was undertaken as part of a programme of study of convulsant and anticonvulsant compounds being carried out in this department.



(I)

Table 1. *Coordinates and isotropic thermal parameters for the refined atoms*

E.s.d.'s are given in parentheses.

	x	y	z	U_{eq}*(Å^2)
C(1)	0·2559 (5)	−0·0090 (3)	0·5193 (1)	0·0535 (23)
C(2)	0·2114 (6)	−0·0892 (3)	0·4873 (2)	0·0649 (27)
C(3)	0·2689 (6)	−0·1813 (3)	0·5028 (2)	0·0655 (26)
C(4)	0·3691 (5)	−0·1914 (2)	0·5501 (1)	0·0497 (22)
C(5)	0·4446 (5)	−0·1839 (2)	0·6766 (1)	0·0408 (20)
C(6)	0·8179 (5)	−0·1115 (2)	0·6376 (1)	0·0459 (22)
C(7)	0·9618 (5)	−0·0576 (3)	0·6499 (2)	0·0531 (25)
C(8)	0·9455 (5)	0·0393 (3)	0·6683 (2)	0·0543 (27)
C(9)	0·7873 (5)	0·0815 (2)	0·6721 (2)	0·0499 (23)
C(10)	0·4656 (4)	0·0714 (2)	0·6600 (1)	0·0419 (21)
C(11)	0·3911 (5)	0·0769 (2)	0·6007 (1)	0·0466 (21)
C(12)	0·3543 (4)	−0·0169 (2)	0·5684 (1)	0·0409 (19)
C(13)	0·4088 (4)	−0·1101 (2)	0·5836 (1)	0·0368 (18)
C(14)	0·6413 (4)	0·0285 (2)	0·6595 (1)	0·0402 (21)
C(15)	0·6596 (5)	−0·0691 (2)	0·6429 (1)	0·0368 (19)
N(1)	0·5365 (5)	−0·1904 (2)	0·7244 (1)	0·0567 (21)
N(5)	0·5089 (3)	−0·1263 (2)	0·6337 (1)	0·0369 (14)
O(1)	0·3079 (3)	−0·2260 (2)	0·6713 (1)	0·0600 (17)
O(10)	0·4752 (4)	0·1681 (2)	0·6829 (1)	0·0644 (18)
H(O10)	0·366 (8)	0·196 (5)	0·678 (3)	0·183 (31)
H(N1)	0·493 (5)	0·268 (3)	0·749 (5)	0·058 (10)
H(N2)	0·347 (5)	0·341 (3)	0·774 (2)	0·080 (14)

* $U_{eq} = (U_{11}U_{22}U_{33})^{1/3}$.

Experimental. Sample provided by Ciba-Geigy Ltd. Colourless prismatic crystals from slow evaporation of ethanol. Crystal 0·2 × 0·3 × 0·5 mm used for data collection, preliminary Weissenberg photographs yielded approximate cell dimensions and showed orthorhombic (*mmm*) Laue symmetry. Space group *Pbca* unambiguously from systematic absences ($0kl$, $k = 2n + 1$; $h0l$, $l = 2n + 1$; $hk0$, $h = 2n + 1$); D_m by flotation (aqueous KI); Enraf–Nonius CAD-4 automated diffractometer, graphite monochromator, Cu $K\alpha$ radiation; 25 high-angle reflections ($25 \leq 2\theta \leq 28°$) used to obtain accurate cell dimensions by least-squares fit; ω–2θ scan width $(0{\cdot}85 + 0{\cdot}15\tan\theta)°$, vertical aperture = 4 mm. 1913 unique reflections measured ($0 \leq h \leq 9$, $0 \leq k \leq 16$, $0 \leq l \leq 28$), 1058 with $I \geq 3\sigma(I)$ ($3 \leq \theta \leq 69°$); three intensity standards ($\bar{1}\bar{5}5$, $\bar{1}\bar{2}8$ and 0,2,13) monitored at intervals of 100 reflections showed no significant variations during data collection; intensity data corrected for Lorentz–polarization factors but no absorption correction applied. Structure solution by direct methods with *SHELX76* (Sheldrick, 1976). Atomic scattering factors from *SHELX76*: *E* map gave positions of the non-H atoms. Refinement by full-matrix least squares with anisotropic thermal factors for all the non-H atoms, isotropic for H atoms, three [H(O10), H(N1) and H(N2)] from difference synthesis, remaining seventeen by calculation, H atoms riding on corresponding C atom (C—H = 1·08 Å); function minimized was $\sum w(|F_o| - |F_c|)^2$, $w = \sum(\sigma^2|F_o| + 0{\cdot}0029|F_c|^2)^{-1}$, $R = 0{\cdot}038$, $wR = 0{\cdot}045$, R (all data) = 0·093, max. (shift/σ) = 0·42 [H(O10)]. Final difference electron density −0·20 to +0·11 e Å^{-3}. Calculations carried out on Amdahl 470V/8 computer. Geometrical calculations performed with *XANADU* (Roberts & Sheldrick, 1975) and molecular illustrations were drawn with *PLUTO* (Motherwell & Clegg, 1978).

Discussion. Atomic coordinates and equivalent isotropic thermal parameters for the refined atoms are given in Table 1.* Molecular geometry is listed in Table 2. The chemical formula with the atomic numbering scheme is shown in (I). Fig. 1 shows a stereoview of the molecular conformation and Fig. 2 shows the crystal packing.

The central azepine ring exists in a twist-boat conformation relative to the plane defined by the atoms C(12), C(13), C(14), C(15). Torsion angles are given in Table 2. The r.m.s. displacement of the four atoms from this plane is 0·10 Å with N(5), C(11) and C(10) lying 0·567, 0·137 and 0·867 Å respectively from the plane. The *N*-carbamoyl group, N(5), C(5), N(1), O(1), is planar with an r.m.s. displacement of 0·003 Å and makes an angle of 3·6 (4)° with the plane defined by C(13), C(15), N(5). The bonds of the azepine ring are in general agreement with the corresponding values reported for 2-morpholinomethyl-5*H*-dibenz[*b,f*]-azepine (Carpy, Gadret, Goursolle, Leger & Lehuede, 1979), 1*H*-azepin-1-yl *p*-bromobenzenesulfonate (Paul, Johnson, Paquette, Barrett & Haluska, 1968) and

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* 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 51568 (8 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Molecular geometry* (Å,°) *for* (I), *e.s.d.'s are in parentheses*

C(12)–C(13)	1·389 (4)	N(5)–C(13)	1·436 (4)
C(13)–C(4)	1·396 (4)	N(5)–C(15)	1·439 (4)
C(4)–C(3)	1·373 (5)	C(15)–C(6)	1·382 (4)
C(3)–C(2)	1·386 (5)	C(6)–C(7)	1·384 (5)
C(2)–C(1)	1·375 (5)	C(7)–C(8)	1·398 (5)
C(1)–C(12)	1·396 (5)	C(8)–C(9)	1·378 (5)
C(12)–C(11)	1·517 (4)	C(9)–C(14)	1·393 (5)
C(11)–C(10)	1·518 (4)	N(5)–C(5)	1·377 (4)
C(10)–C(14)	1·505 (5)	N(1)–C(5)	1·341 (4)
C(14)–C(15)	1·396 (4)	O(1)–C(5)	1·228 (4)
		O(10)–C(10)	1·428 (3)

C(13)–C(12)–C(1)	117·1 (3)	C(5)–N(5)–C(15)	120·3 (3)
C(13)–C(12)–C(11)	125·8 (3)	N(5)–C(5)–O(1)	121·2 (3)
C(1)–C(12)–C(11)	117·1 (3)	N(1)–C(5)–N(5)	116·9 (3)
C(12)–C(13)–C(4)	120·9 (3)	N(1)–C(5)–O(1)	121·9 (3)
C(12)–C(13)–N(5)	121·4 (3)	C(10)–C(14)–C(9)	123·9 (3)
C(4)–C(13)–N(5)	117·7 (3)	C(9)–C(14)–C(15)	118·0 (3)
C(13)–C(4)–C(3)	120·5 (3)	C(14)–C(15)–C(6)	121·3 (3)
C(4)–C(3)–C(2)	119·6 (3)	C(14)–C(15)–N(5)	118·3 (3)
C(3)–C(2)–C(1)	119·6 (3)	C(6)–C(15)–N(5)	120·4 (3)
C(2)–C(1)–C(12)	122·3 (3)	C(15)–C(6)–C(7)	120·0 (3)
C(12)–C(11)–C(10)	119·5 (3)	C(6)–C(7)–C(8)	119·5 (4)
C(11)–C(10)–C(14)	111·6 (3)	C(7)–C(8)–C(9)	119·9 (4)
C(11)–C(10)–O(10)	108·7 (3)	C(8)–C(9)–C(14)	121·2 (3)
C(14)–C(10)–O(10)	108·3 (3)	C(13)–N(5)–C(15)	119·7 (2)
C(10)–C(14)–C(15)	118·0 (3)	C(13)–N(5)–C(5)	119·1 (3)

C(14)–C(10)–C(11)–C(12)	65·3 (4)	C(13)–N(5)–C(15)–C(6)	−108·4 (4)
C(11)–C(10)–C(14)–C(15)	−65·2 (4)	C(4)–C(3)–C(2)–C(1)	0·0 (4)
C(10)–C(14)–C(15)–N(5)	−7·2 (4)	C(2)–C(3)–C(4)–C(13)	2·1 (4)
C(13)–N(5)–C(15)–C(14)	74·2 (4)	C(12)–C(13)–C(4)–C(3)	−2·9 (4)
C(15)–N(5)–C(13)–C(12)	−51·6 (4)	C(4)–C(13)–C(12)–C(1)	1·4 (4)
N(5)–C(13)–C(12)–C(11)	0·0 (4)	C(13)–C(12)–C(1)–C(2)	0·9 (4)
C(10)–C(11)–C(12)–C(13)	−11·9 (4)	C(3)–C(2)–C(1)–C(12)	−1·7 (4)
C(10)–C(11)–C(12)–C(1)	167·6 (4)	C(9)–C(8)–C(7)–C(6)	−2·4 (4)
N(5)–C(13)–C(12)–C(1)	180·0 (4)	C(7)–C(8)–C(9)–C(14)	2·0 (4)
C(4)–C(13)–C(12)–C(11)	−179·1 (4)	C(15)–C(14)–C(9)–C(8)	0·0 (4)
C(15)–N(5)–C(13)–C(4)	127·8 (4)	C(9)–C(14)–C(15)–C(6)	−1·7 (4)
C(11)–C(10)–C(14)–C(9)	111·7 (4)	C14–C(15)–C(6)–C(7)	1·2 (4)
C(9)–C(14)–C(15)–N(5)	175·7 (4)	C(15)–C(6)–C(7)–C(8)	0·0 (4)
C(10)–C(14)–C(15)–C(6)	175·4 (4)		

Hydrogen-bond geometry

D–H···*A*		*D*–H	*D*···*A*	H···*A*	*D*–H···*A*
O(10)–H(O10)···O(1′)	(i)	0·95 (6)	2·675 (7)	1·74 (6)	166 (5)
N(1″)–H(N1″)···O(10)	(ii)	0·88 (6)	2·916 (7)	2·07 (6)	161 (5)

Symmetry code: (i) $\frac{1}{2}-x, \frac{1}{2}+y, z$; (ii) $1-x, \frac{1}{2}+y, 1\frac{1}{2}-z$.

phenyl 1*H*-azepin-1-carboxylate (Linder & von Gross, 1972).

The two phenyl rings [*A* and *B* in (I)] are planar with r.m.s. displacements of 0·010 and 0·009 Å respectively, and no significant deviations from the average bond lengths [*A* = 1·386 (5), *B* = 1·389 (5) Å]. There are, however, three significant deviations from the average bond angle [120·0 (3)°]: C(13)–C(12)–C(1) [117·1 (3)°] and C(9)–C(14)–C(15) [118·0 (3)°] are small (10σ and 7σ) and C(12)–C(1)–C(2) [122·3 (3)°] is large (8σ). The dihedral angle between the two phenyl planes is 127·6 (4)°. The basal plane of the azepine ring, defined by atoms C(12), C(13), C(14) and C(15), makes angles of 162·5 (4) and 35·5 (4)° with rings *A* and *B*, respectively. The centres of the two phenyl moieties lie 4·97 Å apart with N(1) 6·34 and 3·82 Å from the centres of rings *A* and *B*, respectively. Inspection of Fig. 1 reveals that the molecule exhibits distortions from the ideal mirror symmetry of the tricyclic moiety. These distortions are due to the presence of the carboxamide group, the hydroxyl group and to the molecular packing. The packing scheme for GPZ is shown in Fig. 2. Intermolecular hydrogen bonding exists between the amide N (donor) and hydroxyl O (acceptor) atoms and between the hydroxyl O (donor) and carbonyl O (acceptor) atoms. Details are given in Table 2.

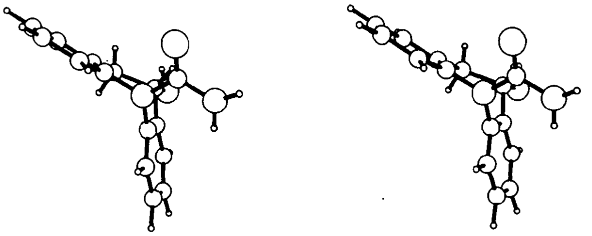

Fig. 1. Stereoview of the molecule along **b**.

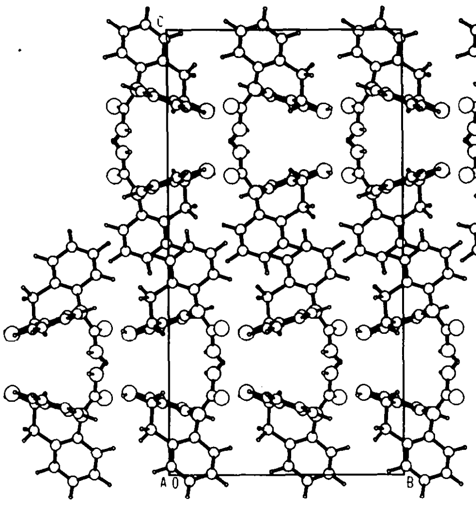

Fig. 2. The crystal structure viewed along **a**.

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