$V = 888\,(1)$ Å^3
$Z = 2$
$D_x = 1.362$ Mg m^{-3}
0.5 × 0.1 × 0.05 mm
Colourless
Crystal source: synthesized at UMIST

Data collection

CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
1887 measured reflections
1638 independent reflections
856 observed reflections [$F > 3\sigma(F)$]
$R_{\text{int}} = 1.36$
$\theta_{\text{max}} = 25.0°$
$h = 0 \rightarrow 6$
$k = 0 \rightarrow 18$
$l = -12 \rightarrow 12$
3 standard reflections monitored every 150 reflections intensity decay: none

Refinement

Refinement on F
$R = 0.0617$
$wR = 0.0701$
$S = 1.649$
856 reflections
244 parameters
H-atom parameters not refined
Weighting scheme based on measured e.s.d.'s
$(\Delta/\sigma)_{\text{max}} = 0.0775$
$\Delta\rho_{\text{max}} = 0.179$ e Å^{-3}
$\Delta\rho_{\text{min}} = -0.191$ e Å^{-3}
Extinction correction: Zachariasen type 2 Gaussian isotropic
Extinction coefficient: $38\,(1) \times 10^{-7}$
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$U_{\text{eq}} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	U_{eq}
O1	0.719 (1)	0.6692	0.5323 (6)	0.051 (3)
N2	0.890 (2)	0.7282 (7)	0.4764 (8)	0.058 (5)
C3	1.111 (2)	0.7185 (9)	0.553 (1)	0.059 (6)
C4	1.096 (2)	0.6271 (8)	0.614 (1)	0.071 (7)
C5	0.863 (2)	0.5898 (8)	0.559 (1)	0.069 (7)
C11	0.899 (2)	0.7191 (8)	0.343 (1)	0.051 (5)
C12	1.079 (2)	0.7620 (9)	0.271 (1)	0.060 (6)
C13	1.076 (2)	0.7613 (10)	0.141 (1)	0.068 (7)
C14	0.886 (3)	0.7182 (10)	0.075 (1)	0.076 (7)
C15	0.720 (2)	0.6748 (9)	0.140 (1)	0.064 (6)
C16	0.721 (2)	0.6765 (9)	0.275 (1)	0.064 (6)
C21	1.143 (2)	0.7896 (8)	0.6487 (10)	0.045 (5)
C22	0.978 (2)	0.8575 (8)	0.6619 (9)	0.048 (5)
C23	1.014 (2)	0.9175 (8)	0.760 (1)	0.058 (6)
C24	1.209 (2)	0.9144 (10)	0.844 (1)	0.067 (7)
C25	1.375 (2)	0.8497 (10)	0.829 (1)	0.075 (7)
C26	1.341 (2)	0.7858 (9)	0.732 (1)	0.069 (7)
C31	0.706 (2)	0.5343 (8)	0.643 (1)	0.057 (6)
C32	0.594 (2)	0.4629 (9)	0.588 (1)	0.061 (6)
C33	0.432 (3)	0.4165 (10)	0.662 (2)	0.088 (9)
C34	0.392 (3)	0.436 (1)	0.783 (2)	0.10 (1)
C35	0.510 (3)	0.504 (1)	0.839 (1)	0.089 (8)
C36	0.661 (3)	0.553 (1)	0.769 (1)	0.086 (9)
F14	0.884 (1)	0.7200 (7)	−0.0539 (7)	0.106 (5)
N23	0.841 (2)	0.9878 (8)	0.769 (1)	0.070 (6)
O23A	0.712 (2)	1.0065 (8)	0.678 (1)	0.097 (6)
O23B	0.823 (2)	1.0234 (8)	0.873 (1)	0.100 (6)

Table 2. *Selected geometric parameters* (Å, °)

O1—N2	1.44 (1)	C3—C4	1.54 (2)
O1—C5	1.49 (1)	C3—C21	1.49 (1)
N2—C3	1.47 (1)	C4—C5	1.52 (2)
N2—C11	1.40 (1)	C5—C31	1.50 (2)
N2—O1—C5	103.4 (7)	N2—C3—C4	105.6 (9)
O1—N2—C3	105.7 (7)	C3—C4—C5	104 (1)
O1—N2—C11	111.6 (8)	O1—C5—C4	102.8 (8)
C3—N2—C11	119.8 (9)		

Data collection: *CAD-4 Diffractometer Control Software* (Enraf–Nonius, 1977). Cell refinement: *CAD-4 Diffractometer Control Software*. Data reduction: *PROCESS TEXSAN* (Molecular Structure Corporation, 1985). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *LS TEXSAN*. Molecular graphics: *ORTEP*II (Johnson, 1976). Software used to prepare material for publication: *FINISH TEXSAN*. Literature search: *CSSR* (1984).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: HU1139). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acta Cryst. (1995). C**51**, 1435–1438

4-(9,10-Dihydro-4*H*-benzo[4,5]cyclohepta[1,2-*b*]thien-4-ylidene)-1-methylpiperidinium Hydrogen Malate†

Oswald M. Peeters, Norbert M. Blaton and Camiel J. De Ranter

Laboratorium voor Analytische Chemie en Medicinale Fysicochemie, Faculteit Farmaceutische Wetenschappen, Katholieke Universiteit Leuven, Van Evenstraat 4, B-3000 Leuven, Belgium

(*Received* 21 *November* 1994; *accepted* 23 *December* 1994)

Abstract

The title compound, $C_{19}H_{22}NS^+.C_4H_5O_5^-$, is a drug used in the treatment of migraine. The tricyclic moiety is asymmetrically folded with a dihedral angle of

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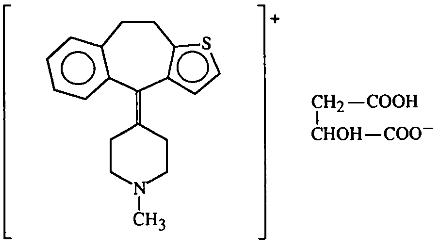
† Internal code of the Janssen Research Foundation: R21448.

Acta Crystallographica Section C
ISSN 0108-2701 ©1995

121.5 (1)° between the aromatic planes. The piperidylidene ring adopts a flattened chair conformation. Hydrogen bonds between symmetry-related malate anions form endless chains in the *a* direction.

Comment

The structure of the title compound (I) has been determined as part of our studies on serotonin antagonists (Blaton, Peeters & De Ranter, 1995, and references therein). Pizotifen (sandomigran, mosegor) is a drug used in the treatment of migraine. Fig. 1 shows a view of the molecule with the hydrogen malate in the *S* configuration. The tricyclic moiety has the common characteristics of dihydrodibenzo[*b*,*f*]heteropins (Blaton, Peeters & De Ranter, 1995). It folds asymmetrically about a line through C4 and C9, the endocyclic angles of the seven-membered ring facing the thiophene ring are markedly enlarged, and the conformation of the central ring is a distorted boat-sofa with a local mirror plane through C11 and the centre of the opposite bond [puckering parameters (Cremer & Pople, 1975) $q_2 = 0.782$ (3), $q_3 = 0.353$ (3) Å, $\varphi_2 = -147.9$ (2), $\varphi_3 = 118.9$ (5)°; asymmetry parameter (Nardelli, 1983*b*) Δ(C11) = 0.056 (1)]. The butterfly angle between the aromatic rings is 121.5 (1)°. This angle decreases with the increasing bulkiness of the double-bonded substituent as can be deduced from the values 145.2 (2)° in DDCHO (Reboul *et al.*, 1983), 131.9 (4)° in IB503 (Bastian & Weber, 1971), 129.3° in noxiptyline (Bandoli & Nicolini, 1983), 114 (3) and 117 (3)° in piroheptine (Tokuma, Nojima & Morimoto, 1968) and 104° in 5-(bromomethylene)-10,11-dihydro-5*H*-dibenzo[*a*,*d*]cycloheptene (Larsson, 1970). The significant difference between the S—C bond distances [1.684 (3) and 1.725 (4) Å] was also found in the IB503 structure. The length of the C4—C15 bond [1.349 (4) Å] indicates an isolated double bond without conjugation with the aromatic rings. The piperidylidene ring has a slightly distorted chair conformation flattened at the C15 apex. The hydrogen malate anion is statistically disordered. Both enantiomers are present at the same position of the unit cell. The conformation of both configurations belongs to type I (van der Sluis & Kroon, 1985). The conformation of the carbon skeleton is antiperiplanar [176.5 (4), −164.6 (8)°] with the carbonyl group of the glycolic acid moiety roughly planar with the hydroxyl O atom [−8.7 (7), −168 (1)°]. O—H···O hydrogen bonds between *a*-glide equivalent malate anions form endless chains in the *a* direction [O29*A*···O26*A*$^{\rm i}$ 2.595 (6); O29*B*···O26*B*$^{\rm i}$ 2.49 (1) Å; symmetry code: (i) $\frac{1}{2} + x$, $-\frac{1}{2} - y$, z]. Within this bridge it is hardly possible to discriminate between the donor and acceptor atom as the electron-density maximum found in a difference Fourier synthesis is situated centrally in a symmetric O—H—O bond. N—H···O hydrogen bonds [N18—H18 0.91, H18···O28*A* 1.84, N18···O28*A* 2.729 Å, N18—H18···O28*A* 165°; H18···O28*B* 2.08, N18···O28*B* 2.961 Å, N18—H18···O28*B* 163°] connect the pizotifen cation to the malate anions.



(I)

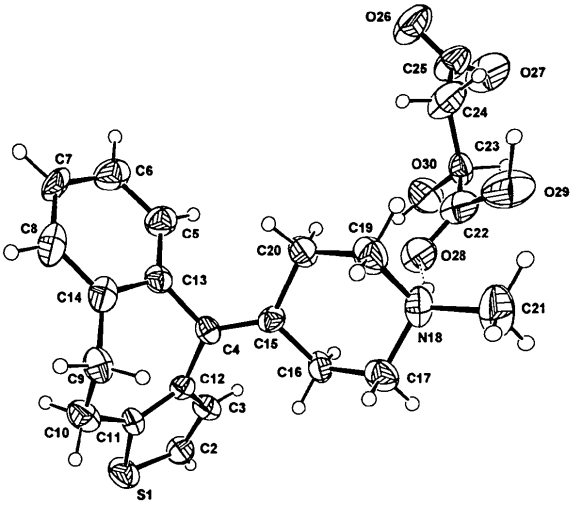


Fig. 1. Perspective view of the title compound with atomic numbering scheme. Displacement ellipsoids are drawn at the 40% probability level.

Experimental

Crystal data

$C_{19}H_{22}NS^+.C_4H_5O_5^-$
$M_r = 429.52$
Orthorhombic
Pcab
$a = 9.973$ (1) Å
$b = 17.101$ (2) Å
$c = 25.496$ (3) Å
$V = 4348.4$ (8) Å^3
$Z = 8$
$D_x = 1.312$ Mg m^{-3}
$D_m = 1.306$ Mg m^{-3}
D_m measured by flotation in *n*-heptane/CCl$_4$

Cu *K*α radiation
$\lambda = 1.54184$ Å
Cell parameters from 24 reflections
$\theta = 20$–25°
$\mu = 1.610$ mm^{-1}
$T = 293$ K
Plate
0.47 × 0.25 × 0.05 mm
Colourless
Crystal source: Janssen Research Foundation, Beerse, Belgium

Data collection

Hilger & Watts four-circle diffractometer
$\omega/2\theta$ scans
Absorption correction: empirical, ψ scan (North, Phillips & Mathews, 1968)
$T_{\min} = 0.757$, $T_{\max} = 0.968$
5220 measured reflections
2773 independent reflections
985 observed reflections $[F^2 > 3.0\sigma(F^2)]$
$R_{\rm int} = 0.0743$
$\theta_{\max} = 56.99°$
$h = 0 \rightarrow 10$
$k = 0 \rightarrow 18$
$l = -26 \rightarrow 26$
4 standard reflections monitored every 50 reflections intensity decay: <3.0%

Refinement

Refinement on F^2
$R[F^2 > 3\sigma(F^2)] = 0.0561$
$wR(F^2) = 0.0909$
$S = 1.415$
2773 reflections
357 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F_o^2) + (0.044P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.085$
$\Delta\rho_{\max} = 0.17$ e Å^{-3}
$\Delta\rho_{\min} = -0.20$ e Å^{-3}
Extinction correction: *SHELXL*93 (Sheldrick, 1993)
Extinction coefficient: 0.00021 (3)
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Tables 2.2B and 2.3.1)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
S1	−0.0222 (1)	0.23145 (6)	0.17320 (4)	0.0743 (4)
C2	−0.1073 (3)	0.2140 (2)	0.2290 (1)	0.059 (2)
C3	−0.0542 (3)	0.1532 (2)	0.2554 (1)	0.054 (1)
C4	0.1312 (3)	0.0497 (2)	0.2540 (1)	0.039 (1)
C5	0.0933 (3)	−0.0878 (2)	0.2233 (1)	0.056 (1)
C6	0.1124 (3)	−0.1462 (2)	0.1860 (1)	0.066 (2)
C7	0.1858 (3)	−0.1329 (2)	0.1412 (1)	0.056 (1)
C8	0.2461 (4)	−0.0603 (2)	0.1351 (1)	0.065 (2)
C9	0.2956 (3)	0.0788 (2)	0.1620 (1)	0.052 (1)
C10	0.1913 (3)	0.1389 (2)	0.1453 (1)	0.061 (2)
C11	0.0890 (3)	0.1563 (2)	0.1853 (1)	0.049 (1)
C12	0.0595 (3)	0.1194 (2)	0.2309 (1)	0.037 (1)
C13	0.1545 (3)	−0.0153 (2)	0.2159 (1)	0.041 (1)
C14	0.2316 (3)	−0.0009 (2)	0.1702 (1)	0.050 (1)
C15	0.1649 (3)	0.0439 (2)	0.3052 (1)	0.039 (1)
C16	0.1382 (3)	0.1073 (2)	0.3452 (1)	0.049 (1)
C17	0.2545 (4)	0.1204 (2)	0.3821 (1)	0.056 (1)
N18	0.2961 (3)	0.0465 (2)	0.40731 (9)	0.051 (1)
C19	0.3377 (3)	−0.0119 (2)	0.3675 (1)	0.057 (1)
C20	0.2249 (3)	−0.0284 (2)	0.3287 (1)	0.051 (1)
C21	0.4032 (3)	0.0593 (2)	0.4471 (1)	0.075 (2)
C22*A*	0.0928 (5)	−0.0712 (3)	0.4726 (2)	0.061 (2)
C23*A*	−0.0142 (5)	−0.1276 (3)	0.4925 (2)	0.053 (2)
C24*A*	0.0195 (6)	−0.2101 (2)	0.4770 (2)	0.077 (2)
C25*A*	−0.0777 (6)	−0.2699 (3)	0.4982 (2)	0.068 (2)
O26*A*	−0.0986 (4)	−0.3276 (2)	0.4672 (2)	0.088 (2)
O27*A*	−0.1331 (4)	−0.2625 (2)	0.5390 (1)	0.098 (2)
O28*A*	0.0627 (4)	−0.0193 (2)	0.4416 (1)	0.074 (2)
O29*A*	0.2076 (4)	−0.0786 (2)	0.4926 (2)	0.086 (2)
O30*A*	−0.1411 (3)	−0.1083 (2)	0.4792 (2)	0.078 (2)
C22*B*	0.106 (1)	−0.0762 (6)	0.4797 (4)	0.061 (3)
C23*B*	0.029 (1)	−0.1432 (5)	0.5045 (3)	0.051 (3)
C24*B*	−0.006 (1)	−0.2046 (5)	0.4647 (4)	0.078 (3)
C25*B*	−0.113 (1)	−0.2604 (6)	0.4847 (5)	0.068 (3)
O26*B*	−0.103 (1)	−0.3297 (5)	0.4673 (4)	0.086 (4)
O27*B*	−0.2041 (9)	−0.2375 (5)	0.5106 (4)	0.130 (6)
O28*B*	0.055 (1)	−0.0388 (5)	0.4436 (3)	0.087 (4)
O29*B*	0.2277 (8)	−0.0702 (5)	0.4922 (4)	0.078 (4)
O30*B*	0.077 (1)	−0.1726 (6)	0.5492 (3)	0.138 (6)

Table 2. *Selected geometric parameters* (Å, °)

S1—C2	1.684 (3)	C17—N18	1.477 (4)
S1—C11	1.725 (4)	N18—C19	1.482 (4)
C2—C3	1.347 (5)	N18—C21	1.490 (4)
C3—C12	1.419 (5)	C19—C20	1.525 (5)
C4—C12	1.509 (4)	C22*A*—C23*A*	1.525 (7)
C4—C13	1.496 (4)	C22*A*—O28*A*	1.225 (6)
C4—C15	1.349 (4)	C22*A*—O29*A*	1.259 (6)
C5—C6	1.391 (5)	C23*A*—C24*A*	1.505 (6)
C5—C13	1.394 (4)	C23*A*—O30*A*	1.351 (6)
C6—C7	1.376 (5)	C24*A*—C25*A*	1.510 (7)
C7—C8	1.388 (5)	C25*A*—O26*A*	1.280 (6)
C8—C14	1.362 (5)	C25*A*—O27*A*	1.185 (6)
C9—C10	1.523 (5)	C22*B*—C23*B*	1.51 (1)
C9—C14	1.519 (5)	C22*B*—O28*B*	1.23 (1)
C10—C11	1.473 (5)	C22*B*—O29*B*	1.26 (1)
C11—C12	1.357 (4)	C23*B*—C24*B*	1.50 (1)
C13—C14	1.417 (5)	C23*B*—O30*B*	1.34 (1)
C15—C16	1.513 (4)	C24*B*—C25*B*	1.52 (1)
C15—C20	1.499 (4)	C25*B*—O26*B*	1.27 (1)
C16—C17	1.510 (5)	C25*B*—O27*B*	1.19 (1)
C2—S1—C11	92.4 (2)	C15—C16—C17	113.0 (3)
S1—C2—C3	111.1 (3)	C16—C17—N18	111.1 (3)
C2—C3—C12	114.2 (3)	C17—N18—C21	111.9 (3)
C13—C4—C15	122.3 (3)	C17—N18—C19	111.0 (2)
C12—C4—C15	123.6 (3)	C19—N18—C21	111.4 (2)
C12—C4—C13	114.0 (3)	N18—C19—C20	111.3 (3)
C6—C5—C13	119.1 (3)	C15—C20—C19	113.7 (3)
C5—C6—C7	121.4 (3)	O28*A*—C22*A*—O29*A*	123.8 (5)
C6—C7—C8	118.1 (3)	C23*A*—C22*A*—O29*A*	116.0 (4)
C7—C8—C14	123.2 (3)	C23*A*—C22*A*—O28*A*	120.1 (4)
C10—C9—C14	110.9 (3)	C22*A*—C23*A*—O30*A*	114.7 (4)
C9—C10—C11	114.6 (3)	C22*A*—C23*A*—C24*A*	110.4 (4)
S1—C11—C10	118.2 (2)	C24*A*—C23*A*—O30*A*	111.9 (4)
C10—C11—C12	130.5 (3)	C23*A*—C24*A*—C25*A*	113.4 (4)
S1—C11—C12	111.2 (3)	C24*A*—C25*A*—O27*A*	122.8 (5)
C4—C12—C11	126.9 (3)	C24*A*—C25*A*—O26*A*	113.9 (4)
C3—C12—C11	111.1 (3)	O26*A*—C25*A*—O27*A*	123.3 (5)
C3—C12—C4	122.0 (3)	O28*B*—C22*B*—O29*B*	123 (1)
C4—C13—C5	120.3 (3)	C23*B*—C22*B*—O29*B*	116.3 (9)
C5—C13—C14	120.2 (3)	C23*B*—C22*B*—O28*B*	119.9 (9)
C4—C13—C14	119.3 (3)	C22*B*—C23*B*—O30*B*	117.4 (9)
C9—C14—C13	119.9 (3)	C22*B*—C23*B*—C24*B*	111.4 (8)
C8—C14—C13	117.9 (3)	C24*B*—C23*B*—O30*B*	113.3 (8)
C8—C14—C9	122.2 (3)	C23*B*—C24*B*—C25*B*	112.2 (8)
C4—C15—C20	123.1 (3)	C24*B*—C25*B*—O27*B*	121.0 (9)
C4—C15—C16	123.7 (3)	C24*B*—C25*B*—O26*B*	114.5 (9)
C16—C15—C20	113.0 (3)	O26*B*—C25*B*—O27*B*	124 (1)
C13—C4—C12—C3	130.1 (3)		
C15—C4—C12—C3	−46.2 (5)		
C12—C4—C13—C14	59.8 (4)		
C15—C4—C13—C5	60.7 (4)		
C12—C4—C13—C5	−115.7 (3)		
C15—C4—C12—C11	135.6 (4)		
C13—C4—C12—C11	−48.0 (4)		
C15—C4—C13—C14	−123.8 (3)		
C10—C9—C14—C8	104.9 (4)		
C10—C9—C14—C13	−75.6 (4)		
C14—C9—C10—C11	65.3 (3)		
C9—C10—C11—S1	172.8 (2)		
C9—C10—C11—C12	−11.8 (5)		
C4—C15—C20—C19	138.9 (3)		
C4—C15—C16—C17	−137.6 (3)		
O28*A*—C22*A*—C23*A*—O30*A*	−8.7 (7)		
O28*A*—C22*A*—C23*A*—C24*A*	118.7 (5)		
O29*A*—C22*A*—C23*A*—O30*A*	166.6 (4)		
O29*A*—C22*A*—C23*A*—C24*A*	−66.0 (6)		
C22*A*—C23*A*—C24*A*—C25*A*	176.5 (4)		
O30*A*—C23*A*—C24*A*—C25*A*	−54.5 (6)		
C23*A*—C24*A*—C25*A*—O26*A*	145.1 (4)		
C23*A*—C24*A*—C25*A*—O27*A*	−32.4 (7)		
O28*B*—C22*B*—C23*B*—O30*B*	−167 (1)		

O28*B*—C22*B*—C23*B*—C24*B*	59 (1)
O29*B*—C22*B*—C23*B*—O30*B*	23 (1)
O29*B*—C22*B*—C23*B*—C24*B*	−109 (1)
C22*B*—C23*B*—C24*B*—C25*B*	−164.6 (8)
O30*B*—C23*B*—C24*B*—C25*B*	60 (1)
C23*B*—C24*B*—C25*B*—O26*B*	−148.0 (9)
C23*B*—C24*B*—C25*B*—O27*B*	39 (1)

Data were collected using a fixed scan speed of 1.2° $\min^{-1}$ and a scan width of 1.2°. Structure solved by Patterson and direct methods for the difference structure. Refinement with full-matrix least squares on F^2 for all reflections. H atoms (except the carboxyl H atom, which was obtained from a difference Fourier synthesis) were calculated at geometrical positions and riding on their parent atom. The hydrogen malate anion was disordered. Both enantiomers are present at the same position and were refined with geometrical and similar U_{ij} restraints (*SADI* and *SIMU* in *SHELXL*93). The sum of the occupancy factors was constrained to 1.0. The occupancy factor for molecule *A* was 0.688 (2).

Data collection: *Y*290 (Hilger & Watts, 1969). Cell refinement: *XRAY*76 (Stewart *et al.*, 1976). Data reduction: *REDU*4 (Stoe & Cie, 1992). Program(s) used to solve structure: *DIRDIF* (Beurskens *et al.*, 1992). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *ORTEX*2.1 (McArdle, 1994). Software used to prepare material for publication: *PARST* (Nardelli, 1983*a*).

The authors thank Dr J. Tollenaere of Janssen Research Foundation (Beerse, Belgium) for providing a sample of the pizotifen malate.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: NA1139). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acta Cryst. (1995). **C51**, 1438–1440

1,3,4,10b-Tetrahydro-4-phenylpyrido[2,1-*a*]isoindole-2,6-dione

Athelstan L. J. Beckwith, Sajan P. Joseph,
Roshan T. A. Mayadunne and Anthony C. Willis

Research School of Chemistry, Institute of Advanced Studies, Australian National University, Canberra, ACT, Australia 0200

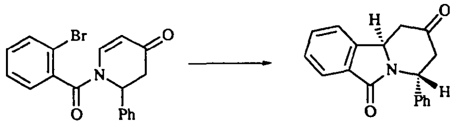
(*Received* 18 *October* 1994; *accepted* 24 *January* 1995)

Abstract

The piperidone ring in the title compound, $C_{18}H_{15}NO_2$, is in a chair conformation. Coordination at the N atom is planar. The phenyl substituent and the bridgehead H atom at the ring junction are *cis* and in axial orientations with respect to the piperidone ring.

Comment

In the course of studies aimed at the diastereoselective synthesis of alkaloids containing the indolizidine nucleus, the substituted dihydropyridone (I) was treated with tributylstannane in benzene to afford (II) as the sole cyclized product (Beckwith, Joseph & Mayadunne, 1993).



(I) (II)

The structure and stereochemistry of (II) were predicted from ^{1}H and ^{13}C NMR spectra, and molecular-mechanics calculations on the transition structure. These predictions have now been validated by the present single-crystal X-ray analysis.

Cremer & Pople (1975) puckering parameters for the piperidone ring, calculated using *RING*88 (Cremer, 1988), indicate that it is in a chair conformation (q_2 = 0.059, q_3 = 0.493 Å, φ_2 = 83.2° and θ_2 = 6.8°). The phenyl substituent at C12 and the H atom at the ring junction (C8) are *cis* and in axial orientations with respect to the piperidone ring, while the C7—C8 bond formed during the cyclization is equatorial. The five-membered ring has a shallow twist conformation