

C7	0.1944 (3)	0.0404 (1)	0.2869 (7)	0.0436
C8	0.1772 (4)	-0.0078 (1)	0.4373 (7)	0.0458
C9	0.2584 (3)	-0.0607 (1)	0.4061 (6)	0.0421
C10	0.3600 (3)	-0.0690 (1)	0.2328 (7)	0.0422
C12	0.4988 (5)	-0.2273 (2)	0.3239 (9)	0.0680
C13	0.5771 (7)	-0.2129 (2)	0.104 (1)	0.1145
C14	0.5500 (5)	-0.1469 (2)	0.0525 (9)	0.0615
C16	0.1338 (6)	0.1432 (2)	0.1601 (9)	0.0643
C17	0.0074 (5)	0.1003 (2)	0.4893 (9)	0.0623

Table 4. Selected geometric parameters (\AA , $^\circ$) for (II)

O1—C2	1.397 (3)	C4—C14	1.493 (5)
O1—C9	1.377 (3)	C5—C6	1.357 (4)
O11—C2	1.212 (4)	C5—C10	1.403 (4)
N15—C7	1.365 (4)	C6—C7	1.412 (4)
N15—C16	1.446 (4)	C7—C8	1.407 (4)
N15—C17	1.434 (5)	C8—C9	1.379 (4)
C2—C3	1.416 (5)	C9—C10	1.388 (4)
C3—C4	1.351 (4)	C12—C13	1.530 (7)
C3—C12	1.507 (4)	C13—C14	1.507 (6)
C4—C10	1.432 (4)		
C2—O1—C9	122.2 (3)	C5—C6—C7	121.7 (3)
C7—N15—C16	121.3 (3)	N15—C7—C6	121.6 (3)
C7—N15—C17	120.9 (3)	N15—C7—C8	121.1 (3)
C16—N15—C17	117.8 (3)	C6—C7—C8	117.3 (3)
O1—C2—O11	115.5 (3)	C7—C8—C9	119.7 (3)
O1—C2—C3	116.6 (3)	O1—C9—C8	115.7 (3)
O11—C2—C3	127.9 (3)	O1—C9—C10	121.1 (2)
C2—C3—C4	121.8 (3)	C8—C9—C10	123.2 (3)
C2—C3—C12	125.8 (3)	C4—C10—C5	126.2 (3)
C4—C3—C12	112.4 (3)	C4—C10—C9	117.2 (3)
C3—C4—C10	121.1 (3)	C5—C10—C9	116.5 (3)
C3—C4—C14	110.8 (3)	C3—C12—C13	102.8 (3)
C10—C4—C14	128.1 (3)	C12—C13—C14	108.0 (4)
C6—C5—C10	121.7 (3)		

For both modifications, weak reflections [$I < 10.0\sigma(I)$] were rescanned (maximum of two rescans) and the counts accumulated to assure good counting statistics. Lp and absorption corrections based on ψ scans were applied; no decay correction. The weighting scheme was based on counting statistics and included a factor ($p = 0.03$) to down weight the intense reflections. Plots of $\sum w(|F_o| - |F_c|)^2$ versus $|F_o|$, reflection order in data collection, $\sin\theta/\lambda$, and various classes of indices showed no unusual trends. The enantiomorphs are indistinguishable from the X-ray data.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1988). Cell refinement: *MSC/AFC Diffractometer Control Software*. Data reduction: *TEXSAN PROCESS* (Molecular Structure Corporation, 1985). Program(s) used to solve structure: *MITHRIL* (Gilmore, 1984). Program(s) used to refine structure: *TEXSAN LS*. Software used to prepare material for publication: *TEXSAN FINISH*. All calculations were performed on a VAXStation 3520 minicomputer.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: CD1037). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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2-[(3,4-Dimethoxybenzyl)(*p*-toluenesulfonyl)amino]-2-phenylethanol

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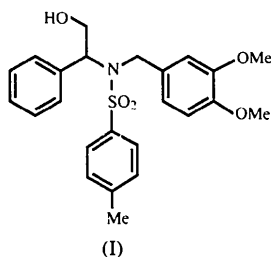
(Received 26 March 1993; accepted 6 April 1994)

Abstract

The crystal structure of the title compound, $C_{24}H_{27}NO_5S$, was determined. The sum of the bond angles around the N atom is 356.6° , showing sp^2 character. The torsion angle N—C(10)—C(17)—O(3) [$-179.0(2)^\circ$] characterizes the antiperiplanar conformation for the N and O atoms. The crystal structure is stabilized by hydrogen bonds [C(9)—H(9)⋯O(4) and C(20)—H(20)⋯O(1)] and van der Waals forces.

Comment

As part of a program of research directed towards the synthesis of nitrogen heterocycles with potential pharmacological activity, we have prepared the title compound (I) by the reaction of 3,4-dimethoxybenzaldehyde and 2-phenyl-2-aminoethanol under reductive amination conditions followed by suitable protection. In our laboratory the amino alcohol derivative (I) was used as precursor in the synthesis of 3-arylisquinoline compounds.



It is well known that protected amino alcohols can be utilized as intermediates in the synthesis of biologically active peptides (Stanfield, Parker & Kanellis, 1981) and optically active amino alcohols are used as drugs, for example Chloramphenicol, and also as components of peptide analogues which function as enzyme inhibitors (Rich, 1985). The determination of the structure of the title compound was undertaken in order to obtain more structural information about amino alcohol derivatives and the effects of substituents in different positions on their conformations.

The N atom in (I) shows sp^2 character as deduced from the sum of its bond angles (356.6°), its displacement from the plane C(1)—C(10)—S (0.164 Å), and the N—S bond distance [1.623 (1) Å] (Cook, Glick, Rigau & Johnson, 1971). The latter value indicates strong double-bond character when compared with the estimated value for single S—N bonds (1.7 Å; Sass,

1960). The N and the O atoms are in an *anti* conformation with a torsion angle N—C(10)—C(17)—O(3) of $-179.0 (2)^\circ$; the distance between the N and O atoms is longer than 5 Å and no O(3)—HO(3)···N hydrogen bond is detected. Nevertheless, a possible weak C(12)—H(12)···O(3) hydrogen bond is observed, compatible with a *gauche* conformation between the phenyl group and the hydroxyl group [C(11)—C(10)—C(17)—O(3) $56.2 (2)^\circ$].

The observed conformation around the C(10)—N bond shows that the tosyl group is eclipsed by the H(10) atom [S—N—C(10)—H(10) $-8 (2)^\circ$], and we can see that the benzyl group attached to the N atom shows *gauche* orientations with respect to the other groups at C(10) as shown by the corresponding torsion angles C(1)—N—C(10)—C(17) $-97.1 (2)^\circ$ and C(1)—N—C(10)—C(11) $30.0 (2)^\circ$.

The two S—O bonds in the present structure possess considerable double-bond character [1.423 (2) and 1.432 (2) Å] (Cruickshank, 1961). The bonding around the S atom is distorted from the ideal tetrahedral geometry. The maximum and minimum values of the bond angles around this atom are O(4)—S—O(5) $119.4 (1)^\circ$ and N—S—O(4) $106.7 (1)^\circ$. The deviation probably results from a stereoelectronic effect. It is noteworthy that the O(4)—S—O(5) angle is larger than the average value for the bond angles in *p*-toluenesulfonyl derivatives (Arora & Sundaralingam, 1971). However, it appears that there are no significant differences from other sulfonamide derivatives (Wdowiak, Gdaniec & Kosturkiewicz, 1990) and the tosyl-L-arginine methyl ester (Barrans & Cotrait, 1976).

The methoxy groups in the dimethoxylated aryl group are approximately coplanar with the benzene nucleus, which is typical for 3,4-dimethoxybenzene derivatives (Arrieta, Badía, Domínguez, Lete, Igartua, Germain, Vlassi & Debaerdemaeker, 1988).

In the unit cell the molecules are stabilized by weak hydrogen bonds [C(9)—H(9)···O(4ⁱ) and C(20)—H(20)···O(1ⁱⁱ); symmetry codes: (i) $x, 1 + y, z$; (ii) $x - 1, y - 1, z$] and van der Waals forces.

Experimental

Crystal data

C₂₄H₂₇NO₅S
 $M_r = 441.55$
 Triclinic
 $P\bar{1}$
 $a = 8.669 (2) \text{ \AA}$
 $b = 10.553 (2) \text{ \AA}$
 $c = 13.535 (3) \text{ \AA}$
 $\alpha = 96.34 (2)^\circ$
 $\beta = 105.91 (3)^\circ$
 $\gamma = 105.02 (2)^\circ$
 $V = 1128.0 (7) \text{ \AA}^3$
 $Z = 2$
 $D_x = 1.300 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation
 $\lambda = 0.71069 \text{ \AA}$
 Cell parameters from 25 reflections
 $\theta = 12\text{--}22^\circ$
 $\mu = 0.181 \text{ mm}^{-1}$
 $T = 298 \text{ K}$
 Prismatic
 $0.2 \times 0.1 \times 0.1 \text{ mm}$
 Colourless

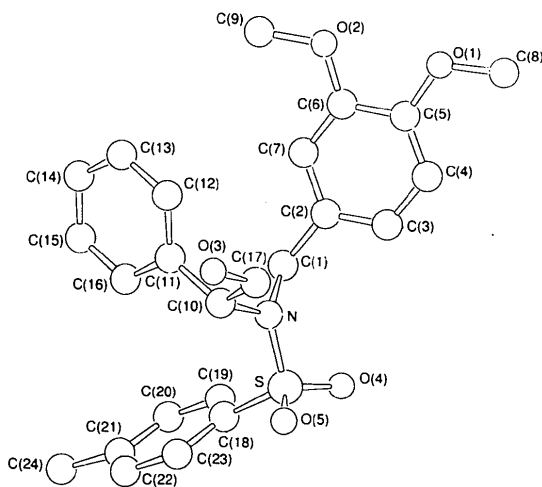


Fig. 1. View of a molecule of (I) showing the labelling of the non-H atoms (SCHAKAL; Keller, 1988).

Data collection
 Enraf-Nonius CAD-4 diffractometer
 $\omega/2\theta$ scans
 Absorption correction: none
 6562 measured reflections
 6562 independent reflections
 4864 observed reflections
 $[I > 2.5\sigma(I)]$

Refinement

Refinement on F^2
 $R = 0.056$
 $wR = 0.066$
 $S = 1.11$
 4864 reflections
 353 parameters
 Only coordinates of H atoms refined
 $w = 1/(\sigma^2|F_o| + 0.005|F_o|^2)$

$\theta_{\max} = 30^\circ$
 $h = -13 \rightarrow 13$
 $k = -16 \rightarrow 16$
 $l = 0 \rightarrow 17$
 3 standard reflections
 frequency: 120 min
 intensity variation: <1%
 $(\Delta/\sigma)_{\max} = 0.1$
 $\Delta\rho_{\max} = 0.3 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.3 \text{ e } \text{\AA}^{-3}$
 Extinction correction: none
 Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

C(6)—O(2)	1.361 (2)	C(16)—C(15)	1.379 (3)
C(9)—O(2)	1.415 (3)	C(19)—C(18)	1.385 (3)
C(17)—O(3)	1.407 (2)	C(23)—C(18)	1.383 (3)
C(2)—C(1)	1.516 (3)	C(20)—C(19)	1.385 (3)
C(3)—C(2)	1.377 (3)	C(21)—C(20)	1.390 (3)
C(7)—C(2)	1.391 (2)	C(22)—C(21)	1.372 (4)
C(4)—C(3)	1.400 (3)	C(24)—C(21)	1.523 (4)
C(5)—C(4)	1.382 (3)	C(23)—C(22)	1.392 (4)
C(6)—C(5)	1.403 (2)		
O(4)—S—N	106.7 (1)	C(6)—C(7)—C(2)	121.2 (2)
O(5)—S—N	106.8 (1)	C(11)—C(10)—N	111.7 (1)
O(5)—S—O(4)	119.4 (1)	C(17)—C(10)—N	107.0 (1)
C(18)—S—N	107.3 (1)	C(17)—C(10)—C(11)	115.3 (2)
C(18)—S—O(4)	109.0 (1)	C(12)—C(11)—C(10)	121.8 (2)
C(18)—S—O(5)	107.1 (1)	C(16)—C(11)—C(10)	119.4 (2)
C(1)—N—S	118.5 (1)	C(16)—C(11)—C(12)	118.8 (2)
C(10)—N—S	117.7 (1)	C(13)—C(12)—C(11)	120.3 (2)
C(10)—N—C(1)	120.4 (1)	C(14)—C(13)—C(12)	119.9 (2)
C(8)—O(1)—C(5)	118.5 (2)	C(15)—C(14)—C(13)	120.3 (2)
C(9)—O(2)—C(6)	116.1 (2)	C(16)—C(15)—C(14)	120.3 (2)
C(2)—C(1)—N	113.7 (1)	C(15)—C(16)—C(11)	120.3 (2)
C(3)—C(2)—C(1)	122.1 (2)	C(10)—C(17)—O(3)	110.2 (2)
C(7)—C(2)—C(1)	119.8 (2)	C(19)—C(18)—S	119.5 (1)
C(7)—C(2)—C(3)	118.0 (2)	C(23)—C(18)—S	120.9 (2)
C(4)—C(3)—C(2)	121.6 (2)	C(23)—C(18)—C(19)	119.4 (2)
C(5)—C(4)—C(3)	120.4 (2)	C(20)—C(19)—C(18)	119.3 (2)
C(4)—C(5)—O(1)	125.7 (2)	C(21)—C(20)—C(19)	122.2 (2)
C(6)—C(5)—O(1)	115.7 (2)	C(22)—C(21)—C(20)	117.3 (2)
C(6)—C(5)—C(4)	118.6 (2)	C(24)—C(21)—C(20)	121.2 (2)
C(5)—C(6)—O(2)	115.0 (2)	C(24)—C(21)—C(22)	121.5 (2)
C(7)—C(6)—O(2)	124.9 (2)	C(23)—C(22)—C(21)	121.7 (2)
C(7)—C(6)—C(5)	120.1 (2)	C(22)—C(23)—C(18)	120.0 (2)

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

$$B_{eq} = (8\pi^2/3) \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	x	y	z	B_{eq}
S	0.18356 (6)	0.76679 (5)	0.29366 (4)	4.02 (2)
N	0.1584 (2)	0.9108 (1)	0.2765 (1)	3.53 (6)
O(1)	0.4266 (2)	1.3326 (2)	0.0009 (1)	4.73 (7)
O(2)	0.1689 (2)	1.3576 (2)	0.0516 (1)	4.79 (7)
O(3)	0.3634 (2)	1.2062 (2)	0.4904 (1)	5.55 (8)
O(4)	0.2076 (2)	0.7087 (2)	0.2005 (1)	5.57 (8)
O(5)	0.3109 (2)	0.7898 (2)	0.3917 (1)	5.66 (8)
C(1)	0.0695 (2)	0.9242 (2)	0.1705 (1)	3.69 (7)
C(2)	0.1720 (2)	1.0325 (2)	0.1291 (1)	3.45 (7)
C(3)	0.3123 (3)	1.0217 (2)	0.1042 (2)	4.48 (9)
C(4)	0.4010 (3)	1.1191 (2)	0.0609 (2)	4.61 (9)
C(5)	0.3498 (2)	1.2304 (2)	0.0429 (1)	3.74 (7)
C(6)	0.2091 (2)	1.2441 (2)	0.0699 (1)	3.49 (7)
C(7)	0.1207 (2)	1.1447 (2)	0.1112 (1)	3.47 (7)
C(8)	0.5641 (5)	1.3217 (4)	-0.0329 (4)	7.09 (18)
C(9)	0.0434 (4)	1.3836 (3)	0.0918 (3)	6.03 (15)
C(10)	0.1709 (2)	1.0069 (2)	0.3706 (1)	3.47 (7)
C(11)	0.0208 (2)	1.0594 (2)	0.3519 (1)	3.61 (7)
C(12)	0.0327 (3)	1.1893 (2)	0.3362 (2)	4.05 (8)
C(13)	-0.1089 (3)	1.2328 (3)	0.3153 (2)	5.08 (11)
C(14)	-0.2624 (3)	1.1471 (3)	0.3105 (2)	5.83 (12)
C(15)	-0.2751 (3)	1.0193 (3)	0.3282 (2)	5.99 (13)
C(16)	-0.1352 (3)	0.9751 (3)	0.3492 (2)	4.89 (10)
C(17)	0.3416 (2)	1.1133 (2)	0.4009 (2)	4.20 (8)
C(18)	-0.0056 (3)	0.6665 (2)	0.3063 (2)	3.82 (7)
C(19)	-0.1453 (3)	0.6116 (2)	0.2181 (2)	4.34 (9)
C(20)	-0.2977 (3)	0.5449 (2)	0.2296 (2)	4.97 (10)
C(21)	-0.3157 (4)	0.5306 (2)	0.3270 (2)	5.31 (11)
C(22)	-0.1747 (4)	0.5836 (3)	0.4130 (2)	5.79 (12)
C(23)	-0.0197 (3)	0.6502 (2)	0.4038 (2)	5.01 (10)
C(24)	-0.4868 (5)	0.4637 (3)	0.3381 (3)	7.96 (18)

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

N—S	1.623 (1)	C(7)—C(6)	1.395 (3)
O(4)—S	1.432 (2)	C(11)—C(10)	1.513 (2)
O(5)—S	1.423 (2)	C(17)—C(10)	1.524 (3)
C(18)—S	1.770 (2)	C(12)—C(11)	1.392 (3)
C(1)—N	1.471 (2)	C(16)—C(11)	1.401 (3)
C(10)—N	1.498 (2)	C(13)—C(12)	1.389 (3)
C(5)—O(1)	1.378 (2)	C(14)—C(13)	1.381 (4)
C(8)—O(1)	1.415 (3)	C(15)—C(14)	1.377 (4)

The positions of three H atoms were calculated and the remaining H atoms were located from a difference Fourier synthesis. The positions of all of the H atoms were refined with an overall isotropic displacement factor, using a riding model for the calculated H atoms.

Data collection: *CAD-4 Software* (Enraf-Nonius, 1989). Cell refinement: *CAD-4 Software*. Program used to solve structure: *SHELXS* (Sheldrick, 1990). Program used to refine structure: *SHELX76* (Sheldrick, 1976). Molecular graphics: *SCHAKAL* (Keller, 1988). Most calculations were performed using *PARST* (Nardelli, 1983).

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Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the IUCr (Reference: HU1057). 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**, 112–114

Methyl (3*R**,4*R**)-4-Hydroxy-3-phenyl-2-(*p*-toluenesulfonyl)-1,2,3,4-tetrahydro-4-isoquinolinylacetate

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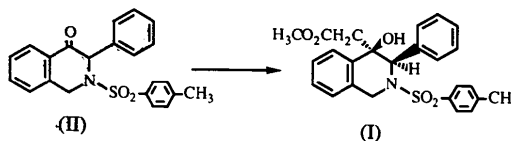
(Received 5 January 1994; accepted 16 May 1994)

Abstract

The X-ray structure analysis of the title compound, C₂₅H₂₅NO₅S, establishes unambiguously the absolute configuration of the asymmetric C atoms as *R* (C9) and *R* C(10), with the hydroxyl and phenyl substituents in *cis* positions. The heterocyclic ring exhibits a flattened sofa conformation. The crystal structure shows an intramolecular hydrogen bond between the hydroxyl group and the carbonyl O atom.

Comment

The benzo[*c*]phenanthridines (Simáneck, 1985) are a family of isoquinoline alkaloids which possess, in many cases, strong pharmacological activity. For example, nitidine and fagaronine are employed for the treatment of some types of leukemia (Sethi, 1985). One of the procedures utilized in organic chemistry for the synthesis of this class of tetracycles involves the use of 3-arylisquinoline derivatives appropriately substituted at the C4 atom. Thus, the title compound (I) has been prepared by applying a typical Reformatsky reaction to a convenient precursor, 4-oxo-3-phenyl-2-(*p*-toluenesulfonyl)-1,2,3,4-tetrahydroisoquinoline (II) (Badía, Domínguez & González-Cameno, 1992). Knowledge of the stereochemistry of derivative (I) appeared interesting with respect to the future preparation of the final benzo[*c*]phenanthridine.



Although NMR spectra and measurements of the difference Nuclear Overhauser Effect (NOE experiments), carried out at ambient temperature in the difference mode by irradiation of all the lines of a multiplet (Hall & Sanders, 1980; Kinns & Sanders, 1984), gave some indication of the stereochemistry of (I), it was not possible to ascertain its exact structure as diagnostic data were not obtained. However, the X-ray analysis was successful in establishing unambiguously the absolute configuration of the target compound as methyl (3*R*,4*R*)-4-hydroxy-3-phenyl-2-(*p*-toluenesulfonyl)-1,2,3,4-tetrahydro-4-isoquinolinylacetate.

A *SCHAKAL* diagram (Keller, 1988) of the title molecule together with the atom-numbering scheme is shown in Fig. 1 and a view of the unit-cell packing is shown in Fig. 2. The molecule consists of an aromatic ring condensed with a hydrogenated heterocyclic ring containing substituents bonded to the asymmetric C9 and C10 atoms and linked to the *p*-toluenesulfonyl group through the N8 atom. The planes of the two rings of the 1,2,3,4-tetrahydroisoquinoline fragment form an angle of 12.07 (8)° with one another and the bond distances and angles are in good agreement with the values reported for other related compounds (Arrieta, Badía, Domínguez, Lete, Igartua, Germain, Vlasi & Debaerdemaeker, 1988; Arrieta, Badía, Domínguez, Lete, Martínez de Marigorta, Germain, Vlasi & Debaerdemaeker, 1988).

The structure of (I) displays a *cis* configuration of the hydroxyl group bonded to the C10 atom and the