Main, P., Fiske, S. J., Hull, S. E., Lessinger, L., Germain, G., Declercq, J.-P. & Woolfson, M. M. (1980). *MULTAN80. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data*. Universities of York, England, and Louvain, Belgium.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Preut, H., Kolev, T., Juchnovski, I. & Bleckmann, P. (1992). *Acta Cryst.* C**48**, 938–940.
Toda, F., Tanaka, K. & Mak, T. C. W. (1985). *Bull. Chem. Soc. Jpn*, **58**, 2221–2227.
Toda, F., Tanaka, K. & Mak, T. C. W. (1988). *Chem. Lett.* pp. 1829–1832.
Zachariasen, W. H. (1963). *Acta Cryst.* **16**, 1139–1144.

Acta Cryst. (1998). C**54**, 954-955

m-(*p*-Tolylsulfonyloxy)aniline

Shyamaprosad Goswami,[a] Ajit Kumar Mahapatra,[b] Gur Dayal Nigam,[c] Kandasamy Chinnakali,[d]† Ibrahim Abdul Razak[d] and Hoong-Kun Fun[d]

[a]*Department of Chemistry, Bengal Engineering College, Botanic Garden, Howrah 711 103, India,* [b]*Department of Chemistry, Indian Institute of Technology, Kharagpur 721 302, West Bengal, India,* [c]*Department of Physics and Meteorology, Indian Institute of Technology, Kharagpur 721 302, West Bengal, India, and* [d]*X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia. E-mail: hkfun@usm.my*

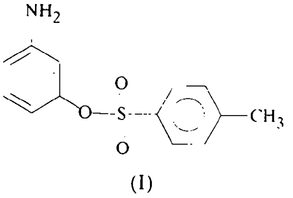
(*Received 8 December 1997; accepted 21 January 1998*)

Abstract

In the title compound, 3-aminophenyl 4-toluenesulfonate, $C_{13}H_{13}NO_3S$, the dihedral angle between the toluene and aniline moieties is 64.26 (5)°. The crystal structure is stabilized by N—H···O intermolecular hydrogen bonds involving amino and sulfonyloxy groups.

Comment

The title compound, (I), is potentially biologically active in mimicking enzyme activity in living organisms. It is expected to show supramolecular behaviour.



(I)

The detailed X-ray structure analysis was undertaken to study the molecular conformation and intermolecular hydrogen-bonding scheme. The S—O and N—C distances, and the mean value of the C—C distances [1.381 (3) Å], agree with the reported values (Allen *et al.*, 1987). The S atom is tetrahedral. The toluene and aniline moieties have a dihedral angle of 64.26 (5)° between them.

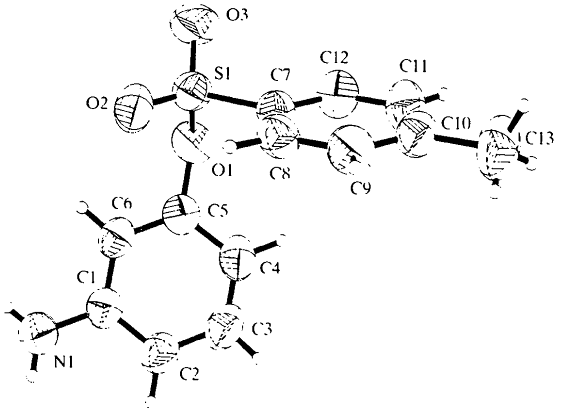


Fig. 1. *SHELXTL/PC* (Sheldrick, 1990) plot of the structure of (I), showing displacement ellipsoids at the 50% probability level and the atom-numbering scheme.

Experimental

To prepare the title compound, *p*-toluenesulfonyl chloride (1 equivalent) was added to a solution of 3-amino-1-hydroxybenzene (1 equivalent) and triethylamine in dry CH_2Cl_2 at 273 K. The reaction mixture was stirred for 15 min at 273 K and 45 min at room temperature. It gave the desired compound in 90% yield (Kurita, 1974). The unreacted compounds were removed by column chromatography, producing a pure sample of (I). Single crystals were grown by slow evaporation of a 1:1 dichloromethane–petroleum ether solution of the compound.

Crystal data

$C_{13}H_{13}NO_3S$
$M_r = 263.30$
Monoclinic
$P2_1/c$
$a = 9.9807$ (7) Å
$b = 7.5585$ (6) Å
$c = 17.0244$ (12) Å
$\beta = 90.196$ (7)°
$V = 1284.3$ (2) Å^3
$Z = 4$
$D_x = 1.362$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 40 reflections
$\theta = 5.41$–12.58°
$\mu = 0.251$ mm^{-1}
$T = 293$ (2) K
Rectangular
0.65 × 0.42 × 0.22 mm
Colourless

Data collection

Siemens *P*4 diffractometer
$\theta/2\theta$ scans

$R_{\rm int} = 0.028$
$\theta_{\rm max} = 27.50$°

---

† On leave from: Department of Physics, Anna University, Chennai 600 025, India.

Acta Crystallographica Section C
ISSN 0108-2701 © 1998

Absorption correction:
empirical ψ scans
(Siemens, 1994)
$T_{\min} = 0.853$, $T_{\max} = 0.939$
3939 measured reflections
2934 independent reflections
1828 reflections with
$I > 2\sigma(I)$

$h = -1 \rightarrow 12$
$k = -1 \rightarrow 9$
$l = -22 \rightarrow 22$
3 standard reflections
every 97 reflections
intensity decay: <3%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.107$
$S = 0.901$
2934 reflections
216 parameters
All H atoms refined
$w = 1/[\sigma^2(F_o^2) + (0.0603P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.266$ e Å^{-3}
$\Delta\rho_{\min} = -0.211$ e Å^{-3}
Extinction correction:
*SHELXL*93
Extinction coefficient:
0.019 (2)
Scattering factors from
International Tables for Crystallography (Vol. C)

Table 1. *Selected bond lengths (Å)*

S1—O2	1.4214 (15)	S1—C7	1.756 (2)
S1—O3	1.4232 (14)	O1—C5	1.431 (2)
S1—O1	1.584 (2)	N1—C1	1.365 (3)

Table 2. *Hydrogen-bonding geometry (Å, °)*

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···O2	0.96 (2)	2.47 (2)	2.901 (2)	107 (1)
N1—H1N1···O3$^{\text{i}}$	0.81 (2)	2.31 (2)	3.098 (3)	165 (2)
N1—H2N1···O2$^{\text{ii}}$	0.79 (3)	2.52 (3)	3.278 (3)	162 (2)

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

The structure was solved by direct methods and refined by full-matrix least-squares techniques. All H atoms were located from a difference Fourier map and refined isotropically.

Data collection: *XSCANS* (Siemens, 1994). Cell refinement: *XSCANS*. Data reduction: *XSCANS*. Program(s) used to solve structure: *SHELXTL/PC* (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *SHELXTL/PC*. Software used to prepare material for publication: *SHELXL*93 and *PARST* (Nardelli, 1995).

The authors would like to thank the Malaysian Government and Universiti Sains Malaysia for research grant R&D No. 190-9609-2801. KC thanks the Universiti Sains Malaysia for a Visiting Postdoctoral Fellowship. AKM is grateful to the Department of Science and Technology, New Delhi, India, for the award of a Senior Research Fellowship.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: HA1211). Services for accessing these data are described at the back of the journal.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans.* 2, pp. S1–S19.
Kurita, K. (1974). *Chem. Ind. (London)*, p. 345.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Sheldrick, G. M. (1990). *SHELXTL/PC Users Manual*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1993). *SHELXL93 Program for the Refinement of Crystal Structures*. University of Göttingen, Germany.
Siemens (1994). *XSCANS Users Manual*. Version 2.1. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Acta Cryst. (1998). C54, 955–957

2-(4-Nitroanilino)-2-phenylethanol

KANDASAMY CHINNAKALI,[a]† HOONG-KUN FUN,[a] KAMARAJ SRIRAGHAVAN[b] AND VAYLAKKAVOOR T. RAMAKRISHNAN[b]

[a]*X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, and* [b]*Department of Organic Chemistry, University of Madras, Guindy Campus, Chennai 600 025, India. E-mail: hkfun@usm.my*

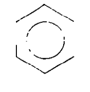
(*Received 5 November 1997; accepted 29 January 1998*)

Abstract

In the title compound, $C_{14}H_{14}N_2O_3$, the nitro group is twisted from coplanarity with the benzene ring by 3.8 (3)°. The benzene ring is perpendicular to the phenyl ring. The molecules are packed around the threefold axis to form an infinite channel containing disordered solvent molecules. C—H···O, O—H···O and N—H···O intermolecular hydrogen bonds stabilize the crystal structure.

Comment

The β-aminoalcohol sequence plays an important role in organic as well as in medicinal chemistry (Goodman & Gilman, 1980). Specifically, the β-amino alcohol subunit has been of particular value in the study of acetylcholine metabolism in intact nerve terminal preparations (Rogers *et al.*, 1989). The crystal structure determination of the title compound, (I), one of the above derivatives, was carried out in order to elucidate the molecular conformation.



(I)

---

† On leave from: Department of Physics, Anna University, Chennai 600 025, India.