Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

p-Phenylene bis(4-methylbenzenesulfonate)

Xiao-Lin Zhang,* Yong-Ping Yan, Wen-Hong Wu, Qun-Sheng Li and Lai-Tao Luo

School of Chemistry and Chemical Industry, Nanchang University, Nanchang 330031, People's Republic of China

Correspondence e-mail: yanyongping6@126.com

Received 29 November 2006
Accepted 6 December 2006

The molecules of the title compound, $C_{20}H_{18}O_6S_2$, lie across centres of inversion. The dihedral angle between the central and terminal benzene rings is 54.92 (9)°.

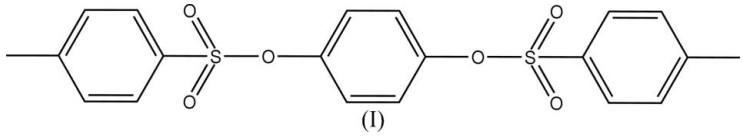
Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.003 Å
R factor = 0.037
wR factor = 0.087
Data-to-parameter ratio = 14.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Sulfonic acid esters exhibit promising efficacy and selectivity against both plasmodium and human skin cancer cells (Betts *et al.*, 2006; Langler *et al.*, 2003). We report here the crystal structure of the title compound, (I).



(I)

The molecule of (I) lies across crystallographic inversion centres. Bond lengths and angles in (I) are normal. The dihedral angle between the C1—C6 and C8—C10/C8^{i}—C10^{i} planes is 54.92 (9)° [symmetry code: (i) 2 − x, −y, 1 − z]. The C1—S1—O3—C8 torsion angle is 57.79 (16)°.

C—H···O intermolecular hydrogen bonds (Table 1) link the molecules into a two-dimensional network parallel to the *bc* plane.

Experimental

Compound (I) was prepared according to the literature method of Manivannan *et al.* (2005*a*,*b*). 4-Toluenesulfonyl chloride (1.0 g) in acetone (4 ml) was added dropwise to a solution of 1,4-dihydroxybenzene (0.26 g) in aqueous NaOH (2.5 ml, 10%), and the mixture was stirred for 10 h. The resulting solid was filtered off and recrystallized from acetone.

Crystal data

$C_{20}H_{18}O_6S_2$
M_r = 418.46
Monoclinic, $P2_1/c$
a = 8.8736 (10) Å
b = 12.3084 (14) Å
c = 9.3696 (10) Å
β = 103.890 (2)°
V = 993.42 (19) Å^3
Z = 2
D_x = 1.399 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.30 mm^{-1}
T = 291 (2) K
Block, colourless
0.35 × 0.25 × 0.20 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.902, T_{max} = 0.942
6050 measured reflections
1819 independent reflections
1127 reflections with $I > 2\sigma(I)$
R_{int} = 0.051
θ_{max} = 25.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.087$
$S = 1.00$
1819 reflections
128 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0406P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10···O2^{ii}	0.93	2.51	3.399 (3)	159

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

H atoms were placed in calculated positions, and refined using a riding model, with C—H = 0.93 or 0.96 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

Thanks are expressed to Huan-Xia Zhang for her help with the crystallographic analysis and the preparation of the paper.

References

Betts, L. M., Tam, N. C., Kabir, S. M. H., Langler, R. F. & Crandall, I. (2006). *Aust. J. Chem.* **59**, 277–282.

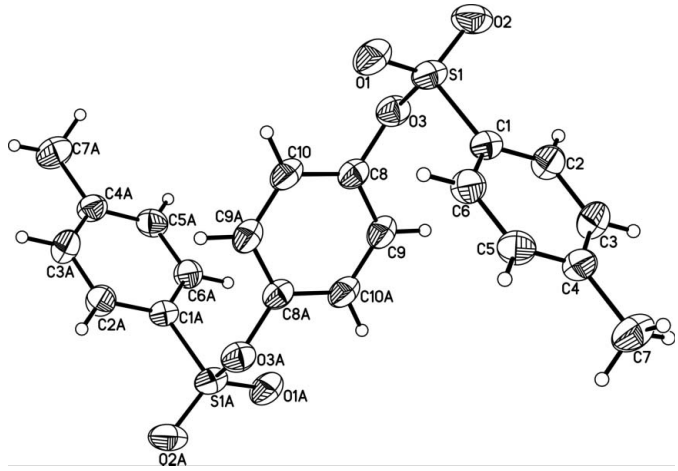


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atomic numbering. Atoms labelled with the suffix A are generated by the symmetry operation $(2-x, -y, 1-z)$.

Bruker (1998). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2005). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Langler, R. F., Paddock, R. L., Thompson, D. B., Crandall, I., Ciach, M. & Kain, K. C. (2003). *Aust. J. Chem.* **56**, 1127–1133.
Manivannan, V., Vembu, N., Nallu, M., Sivakumar, K. & Fronczek, F. R. (2005*a*). *Acta Cryst.* E**61**, o242–o244.
Manivannan, V., Vembu, N., Nallu, M., Sivakumar, K. & Fronczek, F. R. (2005*b*). *Acta Cryst.* E**61**, o75–o78.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.