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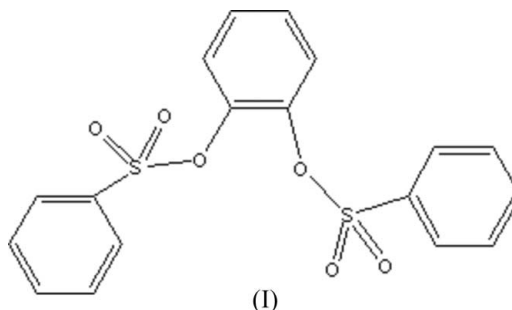
Key indicators

Single-crystal X-ray study
 $T = 294$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.036
 wR factor = 0.093
Data-to-parameter ratio = 15.2For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.*o*-Phenylene bis(benzenesulfonate)

The title molecule, $\text{C}_{18}\text{H}_{14}\text{O}_6\text{S}_2$, adopts an asymmetric conformation with alternating benzene rings and sulfonate groups. In the crystal structure there are two independent $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds, connecting the molecules into a three-dimensional network.

Comment

Sulfonate compounds have important functions in medicine, and as catalysts and acid amplifiers (Hong *et al.*, 2004). Some disulfonate compounds bridged by alkyldiene, alkenyldiene and alkynylidene groups have been reported, such as 2,4-hexadiynylene bis(*p*-methoxybenzenesulfonate) (Fisher *et al.*, 1979), 4,6-decadiynylene bis(pentamethylbenzenesulfonate) (Day *et al.*, 1986), and 2,4-hexadiyne bis(*p*-nitrobenzenesulfonate) (Bertault *et al.*, 1998). In this paper, we report the synthesis and crystal structure of the title compound, (I).



The molecular structure of (I) is illustrated in Fig. 1. The molecule consists of alternating benzene rings and sulfonate groups. The two terminal phenyl rings are not located on the same side of the plane of the central ring, giving an asymmetric conformation. The dihedral angles between the central ring and the terminal ones (C1–C6 and C13–C18) are 48.21 (9) and 48.67 (8)°, respectively, while the dihedral angle between the two terminal phenyl rings is 82.27 (7)°.

In the crystal structure of (I), there are two intermolecular hydrogen bonds (Table 1). $\text{C16}-\text{H16}\cdots\text{O2}^i$ links the molecules into a one-dimensional chain along the *a* axis. These chains are further linked by the $\text{C11}-\text{H11}\cdots\text{O1}^{ii}$ hydrogen bond, resulting in a three-dimensional network (Fig. 2).

Experimental

To a solution of benzenesulfonyl chloride (35.3 g) in dry pyridine (20 ml) and CHCl_3 (50 ml) was added 1,2-benzenediol (11 g) in batches with stirring at about 273–283 K for 6 h. The reaction mixture was poured into ice–water, and the organic layer was separated and washed with water until neutral. The solvent was removed and the

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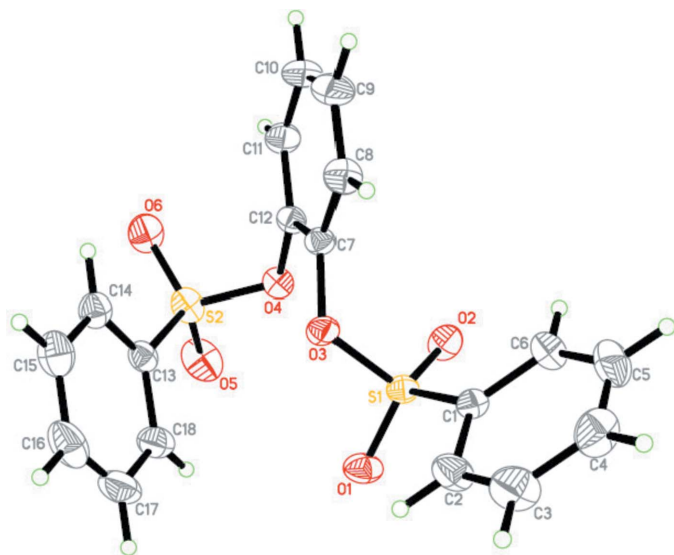


Figure 1
The molecular structure of (I), with the atom-numbering scheme, showing displacement ellipsoids at the 30% probability level.

residue was recrystallized from glycol methyl ether (yield 78%, m.p. 415 K). $^1\text{H NMR}$ (CDCl_3 , p.p.m.): δ 7.802–7.387 (*m*, 1H), 7.714–7.739 (*m*, 2H), 7.612–7.650 (*m*, 2H), 7.365–7.400 (*m*, 1H), 7.198–7.234 (*m*, 2H). Single crystals of the title compound were obtained by slow evaporation of a solution in chloroform/cyclohexane (1:1 *v/v*).

Crystal data

$\text{C}_{18}\text{H}_{14}\text{O}_6\text{S}_2$	$D_x = 1.475 \text{ Mg m}^{-3}$
$M_r = 390.41$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 4019 reflections
$a = 8.8805 (12) \text{ \AA}$	$\theta = 2.8\text{--}26.4^\circ$
$b = 14.404 (2) \text{ \AA}$	$\mu = 0.34 \text{ mm}^{-1}$
$c = 13.754 (2) \text{ \AA}$	$T = 294 (2) \text{ K}$
$\beta = 92.423 (2)^\circ$	Block, colorless
$V = 1757.9 (4) \text{ \AA}^3$	$0.34 \times 0.30 \times 0.14 \text{ mm}$
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	3596 independent reflections
φ and ω scans	2792 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 1997)	$R_{\text{int}} = 0.038$
$T_{\text{min}} = 0.865$, $T_{\text{max}} = 0.954$	$\theta_{\text{max}} = 26.4^\circ$
9780 measured reflections	$h = -11 \rightarrow 5$
	$k = -18 \rightarrow 17$
	$l = -16 \rightarrow 17$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0372P)^2 + 0.6051P]$
$R[F^2 > 2\sigma(F^2)] = 0.036$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.093$	$(\Delta/\sigma)_{\text{max}} = 0.005$
$S = 1.03$	$\Delta\rho_{\text{max}} = 0.30 \text{ e \AA}^{-3}$
3596 reflections	$\Delta\rho_{\text{min}} = -0.36 \text{ e \AA}^{-3}$
236 parameters	Extinction correction: SHELXL97
H-atom parameters constrained	Extinction coefficient: 0.071 (2)

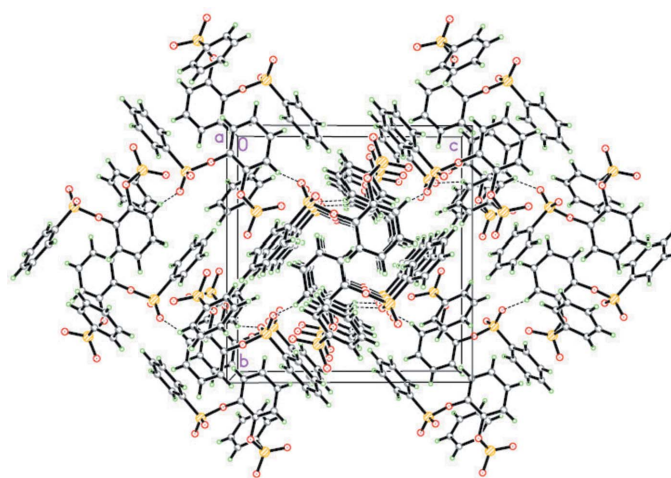


Figure 2
The packing of the molecules, viewed down the *a* axis. Hydrogen bonds are shown as dashed lines.

Table 1

Hydrogen-bond geometry (\AA , $^\circ$).

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
$\text{C16--H16}\cdots\text{O2}^i$	0.93	2.55	3.418 (3)	156
$\text{C11--H11}\cdots\text{O1}^{ii}$	0.93	2.44	3.236 (3)	144

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

All H atoms were initially located in a difference Fourier map. The H atoms were then constrained to an ideal geometry, with C–H distances of 0.93 \AA and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

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

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