

Li Wu, Fu-Xia Liang, Xiao-Ai Sun  
and Wen-Qin Zhang\*Department of Chemistry, Tianjin University,  
Tianjin 300072, People's Republic of China

Correspondence e-mail: wqzhang@tju.edu.cn

## Key indicators

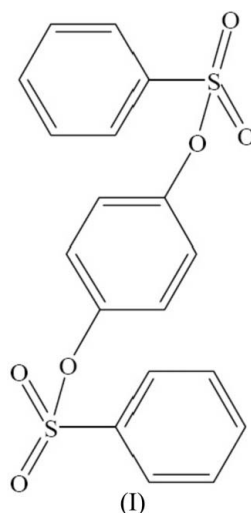
Single-crystal X-ray study  
 $T = 294$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å  
 $R$  factor = 0.043  
 $wR$  factor = 0.121  
Data-to-parameter ratio = 13.5For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.*p*-Phenylene bis(benzenesulfonate)

The title structure,  $\text{C}_{18}\text{H}_{14}\text{O}_6\text{S}_2$ , contains two symmetry-independent conformers. Each conformer resides on a centre of inversion. There are intra- and intermolecular  $\text{C}-\text{H}\cdots\text{O}$  contacts in the structure. The  $\text{C}-\text{S}-\text{O}-\text{C}$  torsion angles are  $-66.6(2)$  and  $-70.0(2)^\circ$  for the two molecules. The bond lengths are normal.

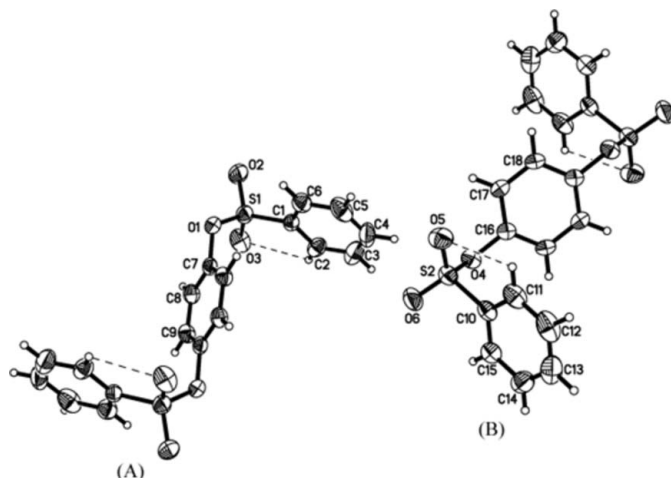
Received 21 August 2006  
Accepted 31 August 2006

## Comment

Sulfonates are becoming increasingly promising since they have been successfully used as photoacid generators in a deep-UV resist system (MacDonald *et al.*, 1994). Nevertheless, until now only a few conformational studies have been carried out (Munro *et al.*, 2003). Sulfonates are flexible due to the presence of the six-valent S atom, with tetrahedral coordination. The molecular constitution offers conformational freedom, which makes the sulfonates an interesting building block in supramolecular chemistry. Recently, we reported the structure of *o*-phenylene bis(benzenesulfonate) (Wu *et al.*, 2005), which adopts an asymmetric conformation with two sulfonate groups and three phenyl rings interlaced alternately.

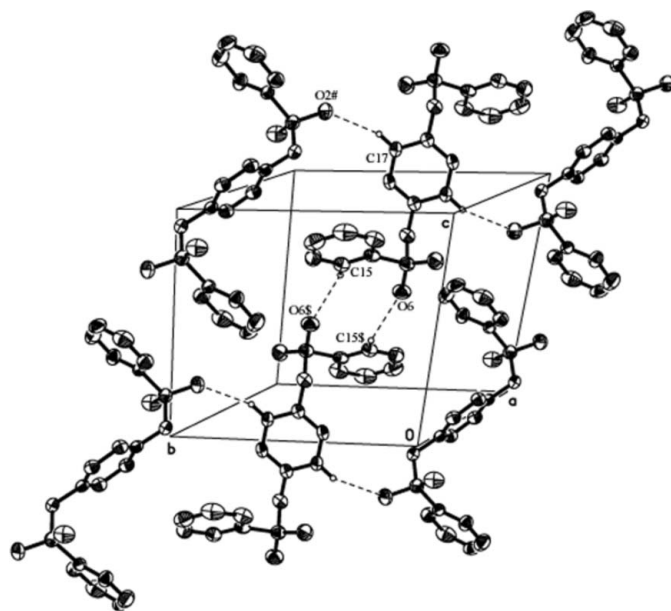


The title molecule, (I), similar to disulfonate compounds bridged by alkylidene, alkenylidene, alkynylidene and naphthalidene groups, such as 2,4-hexadiynylene bis(*p*-methoxybenzenesulfonate) (Fisher *et al.*, 1979), 4,6-decadiynylene bis(pentamethylbenzenesulfonate) (Day *et al.*, 1986), 2,4-hexadiyne bis(*p*-nitrobenzenesulfonate) (Bertault *et al.*, 1998) and 2,7-naphthalenediyl bis(*p*-toluenesulfonate) (Prince *et al.*, 1991), adopts a *Z*-shaped conformation. The crystal structure of (I) displays a variety of inter- and intramolecular contacts



**Figure 1**

The structure of the molecules (A) and (B) of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. Dashed lines indicate the intramolecular hydrogen bonds. In molecule (A) unlabelled atoms are related to labelled atoms by  $1 - x, 2 - y, 2 - z$ . In molecule (B) unlabelled atoms are related to labelled atoms by  $-x, 1 - y, -z$ .



**Figure 2**

Part of the crystal structure of (I), showing the intermolecular hydrogen bonds (dashed lines). For the sake of clarity, H atoms not involved in hydrogen bonding have been omitted. Atoms labelled with a hash (#) or a dollar sign (\$) are at the symmetry positions  $(-x, 2 - y, 1 - z)$  and  $(1 - x, 1 - y, 1 - z)$ , respectively.

There are two independent molecules in the structure of (I). Each molecule resides on a centre of symmetry. The independent molecules are labelled (A) and (B) and are shown in Fig. 1. The respective S—C, S—O and S=O bond lengths of the two conformers are in agreement within the standard uncertainties (Table 1). There is only one pair of significantly different distances, C3—C4 and C4—C5, which are 1.341 (5)

and 1.384 (6) Å, respectively. The C—S—O—C torsion angles are also given in Table 1.

The crystal structure of (I) is stabilized by intermolecular C—H···O hydrogen bonds between molecules (A) and (B), as well as between molecules (B) themselves (Table 2, Fig. 2). There are also intramolecular C—H···O hydrogen bonds (Table 2).

## Experimental

To a solution of benzenesulfonyl chloride (38.8 g, 0.22 mol) in dry pyridine (20 ml) and  $\text{CHCl}_3$  (50 ml) was added 1,4-benzenediol (11 g, 0.1 mol) in batches, while stirring the solution at about 273–283 K for 6 h. The reaction mixture was then poured into ice–water, and the organic layer was separated and washed with water until the pH of the solution was neutral. The solvent was removed and the residue was recrystallized from ethanol (yield 78%, m.p. 388–389 K). IR (KBr):  $1381 \text{ cm}^{-1}$  (O=S=O).

### Crystal data

$\text{C}_{18}\text{H}_{14}\text{O}_6\text{S}_2$

$M_r = 390.41$

Triclinic,  $P\bar{1}$

$a = 8.225$  (2) Å

$b = 10.664$  (3) Å

$c = 12.493$  (3) Å

$\alpha = 101.125$  (4)°

$\beta = 109.046$  (4)°

$\gamma = 110.346$  (4)°

$V = 911.3$  (4) Å<sup>3</sup>

$Z = 2$

$D_x = 1.423 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation

$\mu = 0.32 \text{ mm}^{-1}$

$T = 294$  (2) K

Block, colourless

$0.40 \times 0.34 \times 0.20 \text{ mm}$

### Data collection

Bruker SMART 1000

diffractometer

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(SADABS; Bruker, 1997)

$T_{\min} = 0.862, T_{\max} = 0.937$

4642 measured reflections

3191 independent reflections

2346 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.018$

$\theta_{\max} = 25.0^\circ$

### Refinement

Refinement on  $F^2$

$R[F^2 > 2\sigma(F^2)] = 0.043$

$wR(F^2) = 0.121$

$S = 1.04$

3191 reflections

236 parameters

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0564P)^2$

$+ 0.3203P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.004$

$\Delta\rho_{\max} = 0.21 \text{ e \AA}^{-3}$

$\Delta\rho_{\min} = -0.32 \text{ e \AA}^{-3}$

Extinction correction: *SHELXL97*

(Sheldrick, 1997)

Extinction coefficient: 0.179 (8)

**Table 1**

Selected geometric parameters (Å, °).

S1—O1	1.599 (2)	S2—O4	1.6001 (19)
S1—C1	1.750 (3)	S2—C10	1.748 (3)
O1—S1—C1	103.39 (11)	O4—S2—C10	103.41 (11)
C1—S1—O1—C7	−66.6 (2)	C10—S2—O4—C16	−70.0 (2)

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2 $\cdots$ O3	0.93	2.48	2.875 (4)	106
C11—H11 $\cdots$ O5	0.93	2.58	2.932 (4)	103
C17—H17 $\cdots$ O2 <sup>i</sup>	0.93	2.47	3.329 (5)	154
C15—H15 $\cdots$ O6 <sup>ii</sup>	0.93	2.56	3.274 (5)	134

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

Although all H atoms could be located in a difference Fourier map, they were placed in idealized positions, with aryl C—H distances set to 0.93 Å, and refined as riding, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1997); data reduction: *SAINTE*; 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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