

Jian-Rong Li, Ruo-Hua Zhang
and Xian-He Bu*Department of Chemistry, Nankai University,
Tianjin 300071, People's Republic of China

Correspondence e-mail: buxh@nankai.edu.cn

Key indicators

Single-crystal X-ray study

T = 293 K

Mean $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$

R factor = 0.044

wR factor = 0.115

Data-to-parameter ratio = 16.6

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

1,5-Bis(benzylsulfonyl)pentane

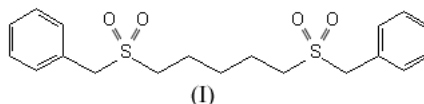
The structure of the title compound, $\text{C}_{19}\text{H}_{24}\text{O}_4\text{S}_2$, shows that the molecular skeleton is extended, with a C_2 axis passing through the central C atom.

Received 6 October 2003

Accepted 10 October 2003

Online 23 October 2003

Comment

Several bis-sulfone compounds, such as (*Z*)-1,2-bis(benzene-sulfonyl)ethylene (Podlaha *et al.*, 1986), *rac*-2,3-bis(ethylsulfonyl)butane (Julia *et al.*, 1986), 1,2-bis(methylsulfonyl)ethane (Mo & Berg, 1982) and bis(phenylsulfonyl)ethane (Hauback & Mo, 1990) *etc.*, were synthesized by the oxidation of their corresponding thioether precursors. In the preparation of a sulfoxide, a sulfone may be obtained because of over-oxidation. During our investigation of disulfoxide ligands, a bis-sulfone, *viz.* 1,5-bis(ethylsulfonyl)pentane, was isolated and structurally characterized (Li *et al.*, 2003). Recently, a similar product, 1,5-bis(benzylsulfonyl)pentane, (I), was obtained.

We report here the crystal structure of (I). The molecular structure is shown in Fig. 1. It can be seen that the chain of atoms linking the two rings is extended, with a C_2 axis passing through the central atom C10 of the molecule; thus the asymmetric unit contains only half of the molecule. All C and S atoms between the two phenyl rings are coplanar, the largest deviation being $0.036(2) \text{ \AA}$ at C8. The four O atoms are located on the same side of the molecular chain formed by the C and S atoms. The dihedral angle between the two sulfonyl planes, O1, S1 and O2 and O1ⁱ, S1ⁱ and O2ⁱ [symmetry code: (i) $-x, y, -z + \frac{1}{2}$], is $1.9(4)^\circ$, and that between the two phenyl rings is $86.7(4)^\circ$. The S=O bond lengths within each SO₂ group are almost equal, with an average value of $1.421(4) \text{ \AA}$, and also essentially equal to that observed in 1,5-bis(ethylsulfonyl)pentane [$1.435(9) \text{ \AA}$]. The average S—C bond length is $1.779(7) \text{ \AA}$ and the average O=S=O angle is $117.4(1)^\circ$.

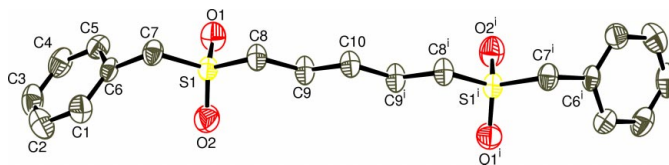


Figure 1
ORTEP-3 (Farrugia, 1997) view of the title compound with the atom-labeling scheme. Ellipsoids are drawn at the 40% probability level [symmetry code: (i) $-x, y, -z + \frac{1}{2}$].

These bond lengths and angles are all within normal ranges and compare well with those observed in other related molecules (Mo & Berg, 1982; Podlaha *et al.*, 1986; Julia *et al.*, 1986; Hauback & Mo, 1990).

Experimental

The title compound was obtained according to a reported procedure for synthesizing disulfoxides (Zhang *et al.*, 1995). Colorless single crystals were obtained by recrystallization from chloroform.

Crystal data

$C_{19}H_{24}O_4S_2$	$D_x = 1.366 \text{ Mg m}^{-3}$
$M_r = 380.50$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 781 reflections
$a = 38.562 (13) \text{ \AA}$	$\theta = 4.3\text{--}25.9^\circ$
$b = 4.7679 (16) \text{ \AA}$	$\mu = 0.31 \text{ mm}^{-1}$
$c = 10.344 (4) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 103.357 (6)^\circ$	Prism, colorless
$V = 1850.3 (11) \text{ \AA}^3$	$0.26 \times 0.24 \times 0.20 \text{ mm}$
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	1889 independent reflections
φ - ω scans	1364 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 1998; Blessing, 1995)	$R_{\text{int}} = 0.032$
$T_{\text{min}} = 0.924$, $T_{\text{max}} = 0.941$	$\theta_{\text{max}} = 26.4^\circ$
5007 measured reflections	$h = -39 \rightarrow 48$
	$k = -5 \rightarrow 5$
	$l = -10 \rightarrow 12$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0587P)^2 + 0.5826P]$
$R[F^2 > 2\sigma(F^2)] = 0.044$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.115$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.04$	$\Delta\rho_{\text{max}} = 0.24 \text{ e \AA}^{-3}$
1889 reflections	$\Delta\rho_{\text{min}} = -0.25 \text{ e \AA}^{-3}$
114 parameters	
H-atom parameters constrained	

Table 1

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

S1—O2	1.4060 (18)	S1—C8	1.772 (2)
S1—O1	1.4368 (18)	S1—C7	1.787 (2)
O2—S1—O1	117.35 (12)	O2—S1—C7	108.59 (11)
O2—S1—C8	108.11 (11)	O1—S1—C7	108.94 (11)
O1—S1—C8	108.36 (11)	C8—S1—C7	104.77 (10)

H atoms were placed geometrically ($C-H = 0.93$ and 0.97 \AA) and refined as riding, with $U_{\text{iso}} = 1.2$ times U_{eq} of the parent atom.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINTE* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL* (Bruker, 1998).

We gratefully acknowledge the financial support of the Outstanding Youth Foundation of NSFC (No. 20225101).

References

- Bruker (1998). *SMART* (Version 5.051), *SAINTE* (Versions 5.01) and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Blessing, R. H. (1995). *Acta Cryst.* **A51**, 33–38.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Hauback, B. C. & Mo, F. (1990). *Z. Kristallogr.* **191**, 195–207.
- Julia, M., Lauron, H., Stacino, J.-P., Verpeaux, J.-N., Jeannin, Y. & Dromzee, Y. (1986). *Tetrahedron*, **42**, 2475–2484.
- Mo, F. & Berg, O. (1982). *Acta Cryst.* **A36**, 657–664.
- Li, J.-R., Zheng, Y., Xie, Y.-B., Zou, R.-Q., Zhang, R.-H. & Bu, X.-H. (2003). *Acta Cryst.* **E59**, o70–o71.
- Podlaha, J., Podlahova, J., Kratochvil, B., Tulsani, N. B., Khawaja, A. M. & Maly, K. (1986). *Acta Cryst.* **C42**, 491–493.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Zhang, R.-H., Zhan, Y.-L. & Chen, J.-T. (1995). *Synth. React. Inorg. Met. Org. Chem.* **25**, 283–292.