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(*R*,*S*)-1,4-Bis(benzylsulfinyl)butane

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

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Key indicators

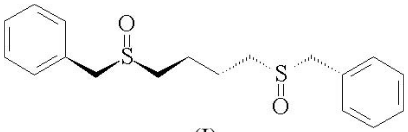
Single-crystal X-ray study
T = 293 K
Mean *σ*(C–C) = 0.007 Å
R factor = 0.068
wR factor = 0.165
Data-to-parameter ratio = 16.1

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

The molecular structure of the title compound, $C_{18}H_{22}O_2S_2$, exhibits an *R,S* configuration for the S atoms. The molecule sits on a centre of symmetry located at the midpoint of the central C—C bond. The C and S atoms between the two phenyl rings are essentially coplanar and make a 87.3 (3)° dihedral angle with the phenyl ring planes.

Comment

Disulfoxides are known to be multifunctional ligands that can coordinate to metal ions *via* either their O or S atoms, depending on electronic and steric factors. The inherent chiral property of the S atom can lead to the formation of diastereomeric *meso* and *rac* isomers. These features make such compounds very interesting ligands for constructing framework complexes. During our investigations of the coordination chemistry of disulfoxides, several ligands of the type RS(O)(CH$_2$)$_n$S(O)R have been structurally determined (Li *et al.*, 2002, 2004; Chen *et al.*, 2001), which exist in diastereoisomeric *rac* or *meso* forms with different melting points.



(I)

As shown in Fig. 1, the title compound, (I), has an *R,S* configuration based on the S atoms. The molecule has a centre of symmetry at the midpoint of the central C—C bond. A similar situation had been observed in (*R,S*)-1,2-bis(methylsulfiny)ethane (Svinning *et al.*, 1976), (*R,S*)-1,2-bis(phenylsulfiny)ethane (Cattalini *et al.*, 1979) and (*R,S*)-1,2-bis(benzylsulfinyl)ethane (Li *et al.*, 2002). All the C and S atoms between the two phenyl rings are almost coplanar, having an average deviation of 0.0287 (3) Å. The two S=O groups lie on opposite sides of the plane and their pseudo-torsion angle (S=O···S=O) is 180°, as required by symmetry. The dihedral angle between this plane and each phenyl ring is 87.3 (3)°. The bond parameters are comparable with the corresponding values for analogous compounds, *viz.*

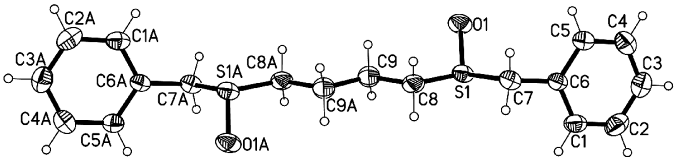


Figure 1
View of the title compound, shown with 50% displacement ellipsoids. Symmetry code: A −*x*, 1 − *y*, 2 − *z*.

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(*R,S*)-1,2-bis(benzylsulfinyl)ethane (Li *et al.*, 2002) and (*R,S*)-1,2-bis(phenylsulfiny)ethane (Cattalini *et al.*, 1979).

Experimental

(R,S)-1,4-Bis(benzylsulfinyl)butane was obtained according to the procedure of Zhang *et al.* (1995) (yield: 40%, m.p: 442–444 K). IR (KBr pellet, cm^{-1}): 3062 (*w*), 3031 (*w*), 2958 (*m*), 2920 (*m*), 2860 (*w*), 1603 (*w*), 1495 (*m*), 1454 (*s*), 1415 (*m*), 1285 (*w*), 1159 (*w*), 1087 (*w*), 1072 (*m*), 1023 (*vs*), 915 (*w*), 889 (*w*), 768 (*s*), 697 (*s*), 670 (*w*), 572 (*w*), 497 (*m*), 431 (*w*); ^{1}H NMR ($CDCl_3$): δ 1.60–1.93 (4H, *m*), 2.55 (4H, *t*), 3.99 (4H, *q*), 7.26–7.28 (4H, *m*), 7.34–7.41 (6H, *m*). Colourless single crystals were obtained by recrystallization from chloroform/methanol (1:1 *v*/*v*).

Crystal data

$C_{18}H_{22}O_2S_2$
$M_r = 334.48$
Monoclinic, $P2_1/c$
$a = 19.382$ (8) Å
$b = 5.303$ (2) Å
$c = 8.492$ (3) Å
$\beta = 93.126$ (6)°
$V = 871.5$ (6) Å^3
$Z = 2$

$D_x = 1.275$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 928 reflections
$\theta = 3.2$–20.0°
$\mu = 0.31$ mm^{-1}
$T = 293$ (2) K
Block, colourless
0.36 × 0.28 × 0.24 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min} = 0.897$, $T_{max} = 0.929$
4306 measured reflections

1611 independent reflections
977 reflections with $I > 2\sigma(I)$
$R_{int} = 0.054$
$\theta_{max} = 25.5°$
$h = -23 \rightarrow 23$
$k = -6 \rightarrow 2$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.069$
$wR(F^2) = 0.165$
$S = 1.03$
1611 reflections
100 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0713P)^2 + 0.483P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.55$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—O1	1.494 (3)	S1—C7	1.806 (4)
S1—C8	1.767 (5)		
O1—S1—C8	105.8 (2)	C8—S1—C7	98.0 (2)
O1—S1—C7	108.4 (2)		

H atoms were placed in calculated positions [C—H = 0.93 and 0.97 Å, and $U_{iso}(H) = 1.2U_{eq}(C)$] and were included in the refinement in the riding-model approximation.

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

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