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(*R*,*R*)-1,3-Bis(phenylsulfinyl)propane

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.044
wR factor = 0.127
Data-to-parameter ratio = 16.9

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

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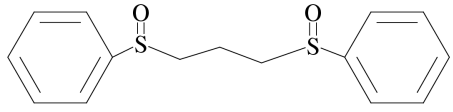
The molecular structure of the title compound, $C_{15}H_{16}O_2S_2$, adopts the *R,R* form. The dihedral angle between the two phenyl rings is 17.4 (2)° and the torsion angle between the two S=O groups is 69.3 (3)°.

Comment

Sulfoxides are of considerable interest because of the potential antitumor activity of their Pt^{II} complexes. Bis-sulfoxide complexes of Pt^{II} are normally *cis* and the antitumor activity depends on the chirality of the ligands (Farrell *et al.*, 1990). There are three isomers with different chirality in bis-sulfoxides, *meso*, (+)-*rac* and (−)-*rac* (Greene *et al.*, 1971). Although the stereoisomers can be characterized by NMR spectroscopy, their molecular structures are less studied (Cattalini *et al.*, 1979). In the present paper, we report the crystal structure of the title compound, namely (*R,R*)-1,3-bis(phenylsulfinyl)propane, (I).



(I)

The molecular structure shown in Fig. 1 has the *R,R* conformation. The dihedral angle between the two phenyl rings is 17.4 (2)° and the torsion angle between the two S=O groups is 69.3 (3)°. A similar situation has been found in the structure of (*R,R*)-1,2-bis(phenylsulphinyl)propane (Cattalini *et al.*, 1979) and there is a close agreement between their geometric parameters.

Experimental

Compound (I) was prepared according to a reported procedure and was characterized by NMR, IR and elemental analyses, giving results consistent with those in the literature (Zhang *et al.*, 1997). Colorless single crystals of the title compound suitable for X-ray diffraction were obtained by slow diffusion of acetone into the chloroform solution of (I).

Crystal data

$C_{15}H_{16}O_2S_2$
M_r = 292.40
Monoclinic, $P2_1/n$
a = 8.444 (4) Å
b = 15.580 (7) Å
c = 11.579 (6) Å
β = 110.333 (9)°
V = 1428.4 (12) Å^3
Z = 4
D_x = 1.360 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6382 reflections
θ = 2.3–26.4°
μ = 0.37 mm^{-1}
T = 293 (2) K
Prism, colorless
0.30 × 0.25 × 0.20 mm

Data collection

Bruker SMART1000 diffractometer	2469 reflections with $I > 2.0\sigma(I)$
ω scans	$R_{int} = 0.026$
Absorption correction: multi-scan [*SAINT* (Bruker, 1998) and *SADABS* (Sheldrick, 1997)]	$\theta_{max} = 26.4^\circ$
	$h = -10 \rightarrow 5$
	$k = -19 \rightarrow 19$
$T_{min} = 0.898$, $T_{max} = 0.930$	$l = -13 \rightarrow 14$
6457 measured reflections	Intensity decay: none
2910 independent reflections	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0643P)^2 + 0.4887P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.044$	
$wR(F^2) = 0.127$	
$S = 1.1$	$(\Delta/\sigma)_{max} < 0.001$
2910 reflections	$\Delta\rho_{max} = 0.75$ e Å^{-3}
172 parameters	$\Delta\rho_{min} = -0.33$ e Å^{-3}
H-atom parameters constrained	Extinction correction: *SHELXL*
	Extinction coefficient: none

The C-bound H atoms were placed in geometrically calculated positions and included in the final refinement in the riding-model approximation with displacement parameters derived from the atoms to which they were bonded.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT*1000 (Bruker, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976).

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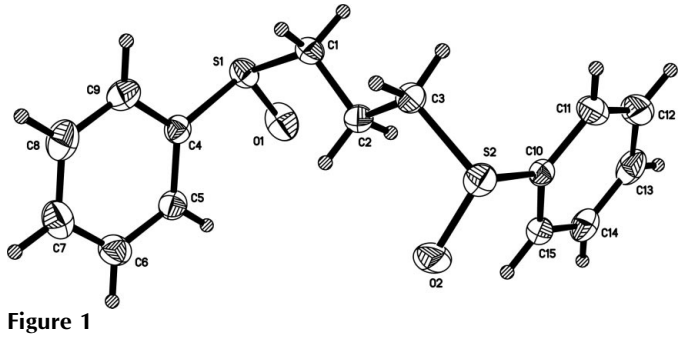

Figure 1
*ORTEP*II (Johnson, 1976) view of the title compound with 30% probability ellipsoids.

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