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1,8-Bis(phenylsulfanyl)octane

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.052
wR factor = 0.132
Data-to-parameter ratio = 18.2

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

The title compound, $C_{20}H_{26}S_2$, crystallizes with two half-molecules in the asymmetric unit. In each independent molecule, there is a centre of inversion at the mid-point of the central C—C bond. Each molecule, excluding H atoms, is roughly planar, and adopts an all-*anti* conformation. The dihedral angles between the phenyl ring and backbone chain are 20.1 (2) and 20.3 (2)°.

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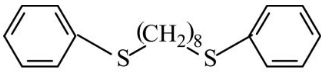
Comment

Since flexible ligands can modify their conformations as a result of changes in the coordination environment (Goodgame *et al.*, 1999), it is interesting to compare the conformations of free ligands with those adopted in their complexes. In the present paper, we report the crystal structure of the title compound, (I), a flexible dithioether ligand (Bpto).



(I)

Compound (I) crystallizes with two half-molecules, *A* and *B*, in the asymmetric unit (Fig. 1). In each independent molecule, there is a centre of inversion at the mid-point of the central C—C bond. Each molecule, excluding H atoms, is roughly planar, and adopts an all-*anti* conformation (Goodgame *et al.*, 1999). The S1···S1*A* and S2···S2*B* distances are 11.703 (2) and 11.749 (4) Å, respectively. The dihedral angles between the phenyl ring and backbone chain are 20.1 (2)° and 20.3 (2)° in molecules *A* and *B*, respectively. A similarly planar all-*anti* ligand conformation is found in silver complexes with 1,4-tris(phenylthio)butane (Bu *et al.*, 2002). In Bpto, the average S—Csp^2 bond distance is 1.754 (2) Å, considerably shorter than the average S—Csp^3 distance of 1.790 (3) Å; corresponding bond distances in several phenylthioether compounds (Murray & Hartley, 1981) are 1.75 and 1.81 Å, respectively. The average C—S—C bond angle, 104.9 (1)°, is within the normal range for thioethers (Blower & Dilworth, 1987) and compares well with that observed in an analogous compound (101.6°; Li *et al.*, 2002).

Experimental

1,8-Bis(phenylthio)octane (Bpto) was prepared according to a reported procedure (Shao *et al.*, 1984), and the product was characterized by NMR, IR and elemental analyses. Colourless single crystals of (I), suitable for X-ray diffraction, were obtained by slow diffusion of acetone into a chloroform solution of Bpto. ^{1}H NMR data ($CDCl_3$, δ, p.p.m.): 1.250 (*t*, 4H), 1.382 (*t*, 4H), 1.610 (*m*, 4H), 2.845 (*t*, 4H), 7.122 (*m*, 10H); FT–IR data (KBr pellet, cm^{-1}): 3440 (*m*), 2921 (*s*), 2850 (*s*), 1479 (*s*), 1437 (*s*), 731 (*s*), 688 (*m*). Analysis calculated for (I) (%): C 72.73, H 7.88; found: C 72.55, H 7.78.

Crystal data

$C_{20}H_{26}S_2$
$M_r = 330.53$
Triclinic, $P\overline{1}$
$a = 5.579$ (2) Å
$b = 7.857$ (3) Å
$c = 20.590$ (7) Å
$\alpha = 84.044$ (5)°
$\beta = 87.890$ (6)°
$\gamma = 89.572$ (6)°
$V = 897.1$ (6) Å^3

$Z = 2$
$D_x = 1.224$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 903 reflections
$\theta = 3.0$–26.3°
$\mu = 0.29$ mm^{-1}
$T = 293$ (2) K
Block, colourless
0.22 × 0.18 × 0.14 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.936$, $T_{\max} = 0.965$
5201 measured reflections

3612 independent reflections
2506 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.023$
$\theta_{\max} = 26.4°$
$h = -5 \rightarrow 6$
$k = -9 \rightarrow 8$
$l = -25 \rightarrow 25$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.132$
$S = 1.04$
3612 reflections
199 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0562P)^2 + 0.209P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.33$ e Å^{-3}
$\Delta\rho_{\min} = -0.21$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C6	1.753 (2)	S2—C16	1.756 (2)
S1—C7	1.787 (3)	S2—C17	1.793 (2)
C6—S1—C7	105.4 (1)	C16—S2—C17	104.5 (1)

All H atoms were positioned geometrically, with Csp^2—H = 0.93 and Csp^3—H = 0.97 Å; they were constrained to ride on their parent atoms with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

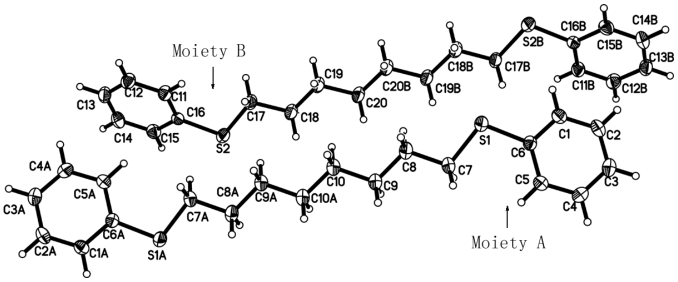


Figure 1
*ORTEP*II (Johnson, 1976) view of the two independent molecules of (I). Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (A) $2 - x, 1 - y, 1 - z$; (*B*) $1 - x, -y, 1 - z$.]

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