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1,4-Bis(phenylsulfanyl)butane

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.060
wR factor = 0.201
Data-to-parameter ratio = 20.1

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

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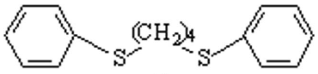
The title compound, $C_{16}H_{18}S_2$, crystallizes with two half-molecules in the asymmetric unit. In each independent molecule, there is a centre of inversion at the mid-point of the central C—C bond. Each molecule, excluding H atoms, is roughly planar and adopts an all-*anti* conformation. The dihedral angles between the phenyl rings and backbone chain are 19.5 (4) and 17.8 (4)°.

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 bisthioether ligand (bptb).



(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 S—C bond distances and C—S—C angles are comparable with those observed in an analogous compound, 1,8-bis(phenylsulfanyl)octane, which has a similar geometry of the alkyl unit (Chen *et al.*, 2004). The S1···S1*A* and S2···S2*B* distances are 6.774 (3) and 6.722 (3) Å, respectively. The dihedral angles between the phenyl ring and the butylene backbone are 19.5 (4) and 17.8 (4)° in molecules *A* and *B*, respectively.

Comparison of the conformation of bptb in (I) and in the silver(I) perchlorate complex with bptb, (II) (Bu *et al.*, 2002), shows some differences. Although a similarly planar all-*anti* alkyl spacer unit is found in (II), the ligand adopts a confor-

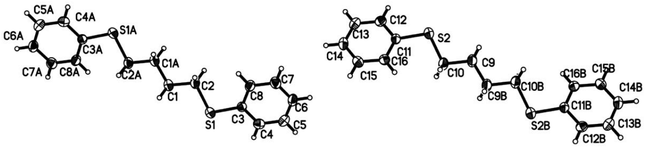


Figure 1
A view of the two independent molecules (*A* left and *B* right) of (I). Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (A) $-x, 2-y, -z$; (B) $1-x, 1-y, 2-z$.]

mation with a slightly longer S···S distance [6.914 (2) Å] and a much larger dihedral angle between the phenyl rings and the backbone chain [91.9 (3)°]. This arrangement may decrease the steric hindrance of ligands around the coordinated Ag^{I}.

Experimental

1,4-Bis(phenylthio)butane (bptb) was prepared according to the procedure reported by 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 evaporation at room temperature of a solution in chloroform. ^{1}H NMR (CDCl$_3$, δ, p.p.m.): 1.78 (*m*, 4H), 2.94 (*t*, 4H), 7.30 (*m*, 10H); FT–IR (KBr pellet, ν, cm^{-1}): 3440 (*m*), 2921 (*s*), 1479 (*m*), 1447 (*m*), 728 (*s*), 683 (*m*). Analysis, calculated for (I): C 70.43, H 6.61%; found: C 70.15, H 6.54%.

Crystal data

$C_{16}H_{18}S_2$
M_r = 274.42
Triclinic, $P\overline{1}$
a = 5.6753 (11) Å
b = 7.7950 (16) Å
c = 16.368 (3) Å
α = 93.02 (3)°
β = 96.00 (3)°
γ = 90.52 (3)°
V = 719.1 (2) Å^3

Z = 2
D_x = 1.267 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7153 reflections
θ = 3.5–27.5°
μ = 0.35 mm^{-1}
T = 293 (2) K
Plate, colourless
0.70 × 0.38 × 0.11 mm

Data collection

Rigaku R-AXIS RAPID imaging-plate diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.705, T_{max} = 0.962
7153 measured reflections

3276 independent reflections
1978 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 27.5°
$h = -7 \rightarrow 6$
$k = -10 \rightarrow 10$
$l = -21 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.201
S = 0.96
3276 reflections
163 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1237P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C3	1.766 (3)	S2—C11	1.759 (3)
S1—C2	1.797 (3)	S2—C10	1.795 (3)
C3—S1—C2	104.38 (13)	C11—S2—C10	104.95 (14)

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

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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