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1,2-Bis(phenylsulfanyl)ethane

Mohamed Osman Awaleh,*
Antonnella Badia and
François Brisse

Département de Chimie, Université de
Montréal, CP 6128, Succ. Centre-ville,
Montréal, Québec, Canada H3C 3J7

Correspondence e-mail:
moawaleh2000@yahoo.fr

Key indicators

Single-crystal X-ray study
T = 220 K
Mean σ(C–C) = 0.002 Å
R factor = 0.036
wR factor = 0.107
Data-to-parameter ratio = 16.0

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

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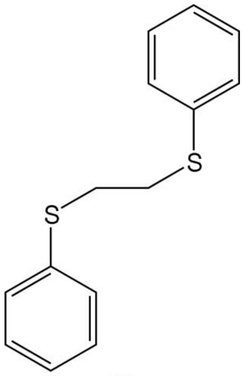
In the title crystal structure, $C_{14}H_{14}S_2$, L^2, the molecules lie on crystallographic inversion centers. The phenyl rings are nearly perpendicular to the planar S—C—C—S group of atoms.

Comment

One of the interests of metal–organic polymer coordination is the design of predictable networks with useful properties (Leininger *et al.*, 2000; Holliday & Mirkin, 2001). Linear bifunctional ligands are often used as building blocks for the construction of metal–organic framework materials (MOF) (Carlucci *et al.*, 2002). The S atom is a soft base and has a good ability to coordinate to silver(I), which is a soft acid. The dithiol group affords two coordination sites to metal centers and can be used to construct supramolecular architectures (Black *et al.*, 1995; Bu *et al.*, 2002). We report here the structure of 1,2-bis(phenylsulfanyl)ethane, L^2, (I).



(I)

The molecular structure of (I) is shown in Fig. 1. There is a crystallographic center of symmetry at the midpoint of the central C—C bond. Hence, the torsion angle S1—C7—C7^i—S1^i is 180° [symmetry code: (i) $2 - x, -y, 1 - z$]. The C1—S1—C7—C7^i torsion angle is 83.9 (2)°, and thus the aliphatic segment (S—CH$_2$—CH$_2$—S) is nearly perpendicular to the phenyl rings. In contrast, the longer chain molecule 1,10-bis(phenylsulfanyl)decane, L^{10}, is nearly wholly planar (Awaleh *et al.*, 2005). The bond distances and angles in L^2 are in the normal range (Table 1) (*International Tables for Crystallography*, 1995, Vol. C).

In the crystal packing of (I), illustrated in Fig. 2, there are no significant π–π stacking interactions. The S$\cdots$S distance between adjacent molecules, with a value of 3.5136 (8) Å, is slightly less than the sum of the van der Waals radii (3.60 Å; Porterfield, 1994). These short contacts are shown in Fig. 3.

Another determination of the title compound is reported in the following paper (Hou *et al.*, 2005).

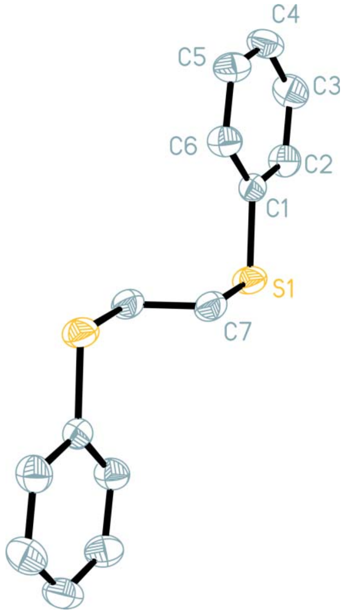


Figure 1
The molecular structure and atomic numbering of (I). Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted. The unlabeled part of the molecule is related by the symmetry transformation ($2 - x$, $-y$, $1 - z$).

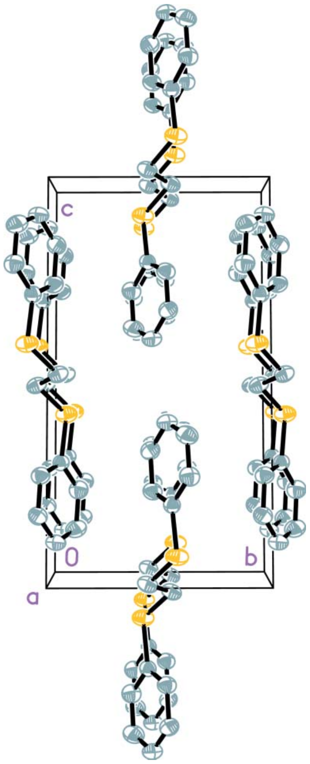


Figure 2
A crystal packing diagram of (I), viewed along the *a* axis. H atoms have been omitted.

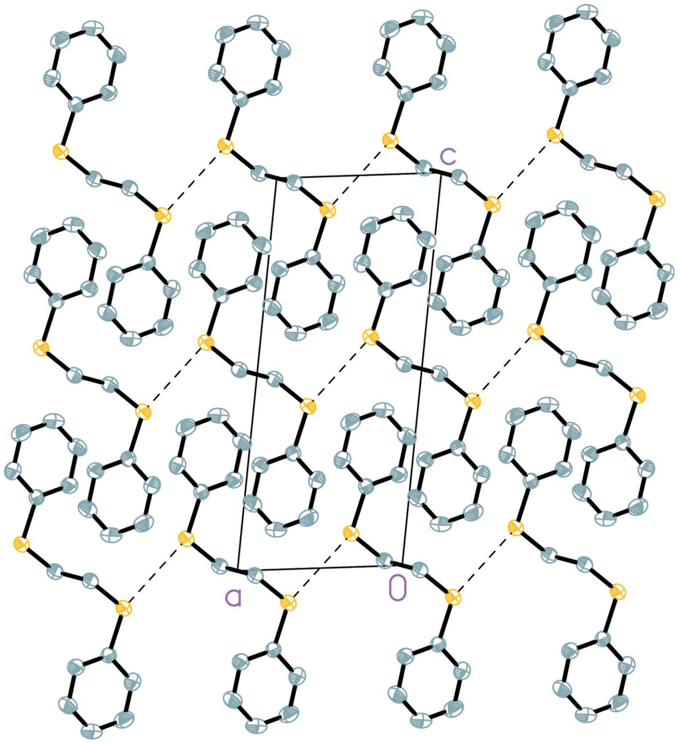


Figure 3
A packing diagram, showing the S···S short contacts (dashed lines) between adjacent L^2 molecules. H atoms have been omitted.

Experimental

The title compound was synthesized according to the published procedure of Hartley *et al.* (1979). The ^{1}H NMR spectrum, recorded in acetone-d_6, confirms the purity of the compound. Compound (I) was obtained as a crystalline powder from which a needle-like crystal suitable for X-ray analysis was isolated (yield 43%). Analysis, found: C 68.25, H 6.09%; calculated for $C_{14}H_{14}S_2$: C 68.24, H 5.73%. ^{1}H NMR (acetone-d_6 δ, p.p.m.): 3.14 [*s*, 4H, –S-(CH_2)$_2$-S–], 7.32 (*m*, 10H, C_6H_5–).

Crystal data

$C_{14}H_{14}S_2$
$M_r = 246.37$
Monoclinic, $P2_1/c$
$a = 5.8654$ (1) Å
$b = 7.5638$ (1) Å
$c = 14.0472$ (2) Å
$\beta = 97.600$ (1)°
$V = 617.73$ (2) Å^3
$Z = 2$

$D_x = 1.325$ Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 4189 reflections
$\theta = 3.2$–$72.7°$
$\mu = 3.63$ mm^{-1}
$T = 220$ (2) K
Needle, colorless
0.32 × 0.06 × 0.05 mm

Data collection

Bruker SMART 2000 area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick,1996)
$T_{\min} = 0.375$, $T_{\max} = 0.825$
5018 measured reflections

1184 independent reflections
1099 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.026$
$\theta_{\max} = 72.7°$
$h = -5 \rightarrow 6$
$k = -9 \rightarrow 9$
$l = -17 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.107$
$S = 1.03$
1184 reflections
74 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0794P)^2 + 0.1086P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.23$ e Å^{-3}
$\Delta\rho_{\min} = -0.23$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.018 (2)

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Table 1
Selected geometric parameters (Å, °).

S1—C1	1.7667 (15)	C7—C7^{i}	1.515 (3)
S1—C7	1.8123 (16)		
C1—S1—C7	105.08 (7)	C7^{i}—C7—S1	112.48 (14)
C1—S1—C7—C7^{i}	83.90 (17)		

Symmetry code: (i) $2 - x, -y, 1 - z$.

H atoms were placed in calculated positions (C—H = 0.93–0.98 Å) and refined as riding atoms, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C). A final verification of possible voids was performed using the VOID routine of the *PLATON* program (Spek, 2003).

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *UdMX* (Maris, 2004).

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