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Key indicators

Single-crystal X-ray study
T = 293 K
Mean $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$
R factor = 0.042
wR factor = 0.131
Data-to-parameter ratio = 19.2

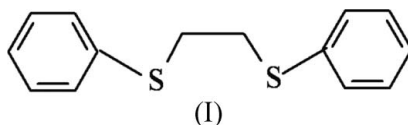
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

1,2-Bis(phenylsulfanyl)ethane

In the title compound, $\text{C}_{14}\text{H}_{14}\text{S}_2$, there is a centre of inversion at the mid-point of the central C—C bond. Excluding H atoms, the molecule adopts an anti conformation, with a planar $-\text{S}-\text{CH}_2-\text{CH}_2-\text{S}-$ spacer unit. The dihedral angle between the phenyl ring and the S—C—C—S chain is $84.52(18)^\circ$.

Comment

Many complexes of bis(thioether) ligands with transition metal ions, such as silver(I) (Black *et al.*, 1995), palladium(II) (Errington *et al.*, 1980) and platinum(II) (Murray & Hartley, 1981), have been characterized and have interesting structures. In contrast, the structures of the free ligands have been much less studied. In the present paper, we report the crystal structure of the title compound, a bis(thioether) ligand, *viz.* 1,2-bis(phenylsulfanyl)ethane (bpte), (I).



The bpte molecule has a centre of inversion at the mid-point of the central C1—C1A bond; symmetry code: (A) $1 - x, -y, -z$; Fig. 1]. Excluding H atoms, the molecule adopts an anti conformation (Goodgame *et al.*, 1999), with a planar spacer unit (S1—C1—C1A—S1A). The S—C bond distances and C—S—C angles are comparable to those observed in an analogous compound, 1,4-bis(phenylsulfanyl)butane (Chen *et al.*, 2005). The S1...S1A non-bonded distance is $4.4223(16) \text{ \AA}$. The phenyl ring makes a dihedral angle of $84.52(18)^\circ$ with the plane of the spacer unit (S1—C1—C1A—S1A).

In the crystal structure of the silver(I) nitrate complex with bpte, (II) (Shao *et al.*, 1991), the ligand adopts a different geometry; the orientation of one phenyl group of bpte with respect to the spacer plane is similar to that in the title

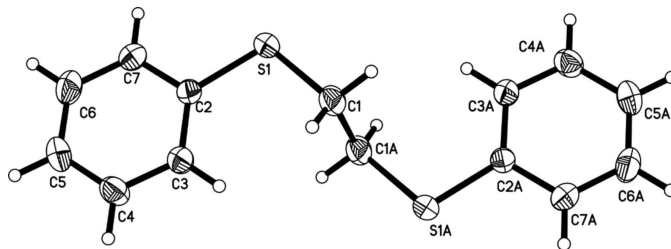


Figure 1
ORTEP (Johnson, 1976) view of the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (A) $1 - x, -y, -z$.]

compound, but the other phenyl group is twisted about the S—C_{phenyl} bond. There is no centre of symmetry and the phenyl rings are inclined to each other by 63.4°. A similar torsion can also be found in the PdCl₂ complex with bpte, (III) (Wang *et al.*, 1992).

The S—C bond length and S··S non-bonded distance in free bpte are slightly shorter than those in complexes (II) and (III), and other analogous bis(thioethers) and corresponding complexes (Bu *et al.*, 2002).

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

Experimental

1,2-Bis(phenylsulfanyl)ethane (bpte) was prepared according to a reported procedure (Shao *et al.*, 1991) and the product was characterized by NMR. Colourless single crystals of the title compound, suitable for X-ray diffraction, were obtained by slow evaporation at room temperature of a solution in chloroform. ¹H NMR (CDCl₃): δ 3.02 (t, 4 H), 7.36 (m, 10 H).

Crystal data

C ₁₄ H ₁₄ S ₂	$D_x = 1.303 \text{ Mg m}^{-3}$
$M_r = 246.39$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 5725 reflections
$a = 5.8389 (12) \text{ \AA}$	$\theta = 3.0\text{--}27.5^\circ$
$b = 7.6865 (15) \text{ \AA}$	$\mu = 0.39 \text{ mm}^{-1}$
$c = 14.124 (3) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 97.90 (3)^\circ$	Needle, colourless
$V = 627.9 (2) \text{ \AA}^3$	$0.80 \times 0.23 \times 0.10 \text{ mm}$
$Z = 2$	

Data collection

Rigaku R-AXIS RAPID IP area-detector diffractometer	1418 independent reflections
ω scans	1180 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$R_{\text{int}} = 0.058$
$T_{\text{min}} = 0.745$, $T_{\text{max}} = 0.961$	$\theta_{\text{max}} = 27.5^\circ$
5725 measured reflections	$h = -6 \rightarrow 7$
	$k = -9 \rightarrow 9$
	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0735P)^2 + 0.1339P]$
$R[F^2 > 2\sigma(F^2)] = 0.042$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.131$	$(\Delta\sigma)_{\text{max}} < 0.001$
$S = 1.03$	$\Delta\rho_{\text{max}} = 0.48 \text{ e \AA}^{-3}$
1418 reflections	$\Delta\rho_{\text{min}} = -0.28 \text{ e \AA}^{-3}$
74 parameters	Extinction correction: SHELXL97
H-atom parameters constrained	Extinction coefficient: 0.059 (13)

Table 1

Selected geometric parameters (\AA , $^\circ$).

S1—C2	1.7609 (17)	S1—C1	1.825 (2)
C2—S1—C1	105.15 (9)		

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

Data collection: RAPID-AUTO (Rigaku, 2004); cell refinement: RAPID-AUTO; data reduction: RAPID-AUTO; 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: CrystalStructure (Rigaku, 2004).

We gratefully acknowledge financial support from the National Natural Science Foundation of China (No. 20206022).

References

- Awaleh, M. O., Badia, A. & Brisse, F. (2005). *Acta Cryst.* **E61**, o2479–o2480.
- Black, J. R., Champness, N. R., Levason, W. & Reid, G. (1995). *J. Chem. Soc. Chem. Commun.* pp. 1277–1278.
- Bu, X.-H., Chen, W., Hou, W.-F., Du, M., Zhang, R.-H. & Brisse, F. (2002). *Inorg. Chem.* **41**, 3477–3482.
- Chen, W., Hou, B.-H., Zhou, L.-N., Wang, J.-K. & Li H. (2005). *Acta Cryst.* **E61**, o1890–o1891.
- Errington, J., McDonald, W. S. & Shaw, B. L. (1980). *J. Chem. Soc. Dalton Trans.* pp. 2309–2315.
- Goodgame, D. M. L., Grachvogel, D. A., Hussain, I., White, A. J. P. & Williams, D. J. (1999). *Inorg. Chem.* **38**, 2057–2063.
- Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
- Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
- Murray, S. G. & Hartley, F. R. (1981). *Chem. Rev.* **81**, 365–414.
- Rigaku. (2004). RAPID AUTO and *CrystalStructure*. Rigaku/MSI Inc., 9009 New Trails Drive, The Woodlands, TX 77381-5209, USA.
- Shao, P.-X., Yao, X.-K., Wang, H.-G., Wang, W.-H., Liu, B., Li, M., Luo, L.-W. & Xu D.-H. (1991). *Chem. J. Chin. Univ.* **12**, 143–147.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Wang, W.-Z., Shao, P.-X., Yao, X.-K., Wang, R.-J. & Wang, H.-G. (1992). *J. Struct. Chem.* **11**, 17–19.