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4,4′-Bis[(phenylsulfanyl)methyl]biphenyl

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Key indicators

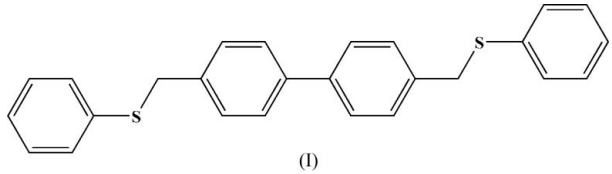
Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.003 Å
R factor = 0.036
wR factor = 0.098
Data-to-parameter ratio = 14.3

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

The title compound, $C_{26}H_{22}S_2$, was obtained by the reaction of 4,4′-bis(chloromethyl)biphenyl with the sodium salt of thiophenol in ethanol. The molecule has an inversion centre, with the two phenyl fragments in the same plane.

Comment

The rational design of coordination architectures based on multitopic organic ligands and metal centres represents one of the most rapidly developing fields in current coordination and supramolecular chemistry owing to their fascinating structures and their potential as functional materials (Yaghi *et al.*, 2003; Zheng *et al.*, 2003; Kitagawa *et al.*, 2004). Recently, we synthesized the new semirigid dithioether ligand, (I), and we report here its crystal structure.



(I)

As shown in Fig. 1, the molecule of (I) has an inversion centre at the mid-point of the central C—C bond, with the two phenyl fragments in the same plane. The C6—S1 [1.7682 (2) Å] and C7—S1 [1.8015 (2) Å] bonds and C6—S1—C7 [103.72 (8)°] and S1—C7—C8 [108.72 (1)°] angles are all in normal ranges, and comparable with the corresponding values in other analogues (Allen *et al.*, 1987; Casabó *et al.* 1995). The dihedral angle between the C1–C6 and C8–C13 rings is 64.20 (3)°.

Experimental

The title compound was prepared according to a literature method (Mikhailov *et al.*, 1984). 4,4′-Bis(chloromethyl)biphenyl (2.51 g, 10 mmol) was added dropwise to a hot solution (about 333 K) of the thiophenol sodium salt (2.64 g, 20 mmol) in ethanol (40 ml), and the

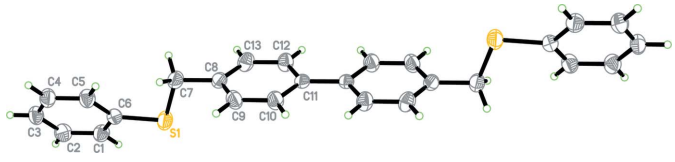


Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Unlabelled atoms are related to labelled atoms by the symmetry operation $(-x, 1-y, 1-z)$.

mixture was stirred at 333 K for a further 6 h. After cooling, water (30 ml) was added and the mixture was allowed to stand for 2 h. The resulting yellow precipitate was filtered off, washed with ethanol and water, and then recrystallized from a mixture of chloroform and methanol (1:1), giving single crystals suitable for X-ray diffraction analysis (yield 3.60 g, 90%).

Crystal data

$C_{26}H_{22}S_2$
M_r = 398.58
Monoclinic, $P2_1/c$
a = 23.2051 (6) Å
b = 5.5097 (1) Å
c = 8.0412 (2) Å
β = 91.216 (2)°
V = 1027.86 (4) Å^3
Z = 2
D_x = 1.288 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.27 mm^{-1}
T = 273 (2) K
Block, yellow
0.24 × 0.22 × 0.22 mm

Data collection

Bruker APEX-II CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.939, T_{max} = 0.943
8768 measured reflections
1815 independent reflections
1393 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.098
S = 1.04
1815 reflections
127 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0466P)^2 + 0.2242P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

H atoms were positioned geometrically, with C—H = 0.93 and 0.97 Å for aromatic and methylene H atoms, respectively and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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, 1998); software used to prepare material for publication: *SHELXTL*.

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