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9,10-Bis[(phenylsulfanyl)methyl]anthracene

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Key indicators

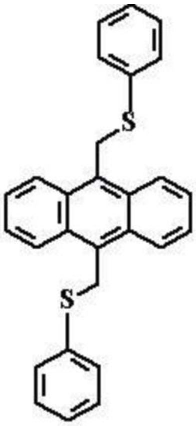
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.040
wR factor = 0.100
Data-to-parameter ratio = 16.3

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

The title compound, $C_{28}H_{22}S_2$, was obtained by the reaction of 9,10-bis(chloromethyl)anthracene with the sodium salt of thiophenol in ethanol. The molecule has an inversion centre, with the two phenyl fragments in the same plane; this plane is approximately orthogonal to the anthracene plane [dihedral angle = 99.5 (7)°].

Comment

The design and syntheses of flexible multi-thioether ligands have attracted much attention due to their diverse coordination capabilities and the important properties of their metal complexes (Li *et al.*, 2003; Xie *et al.*, 2004). Recently, we synthesized a new dithioether ligand, namely 9,10-bis[(phenylsulfanyl)methyl]anthracene, (I). We report here the crystal structure of this dithioether ligand.



(I)

As shown in Fig. 1, the molecule of (I) has an inversion centre, with the two phenyl fragments located on different sides of the anthracene plane; thus the asymmetric unit contains only half of the molecule. The two phenyl fragments are in the same plane, which is approximately orthogonal to the anthracene plane, with a dihedral angle of 99.5 (7)°. The two C—S bonds, *viz*. C1—S1 and C7—S1, are 1.766 (2) and 1.811 (2) Å, respectively. The angles C10—C7—S1 and C1—S1—C7 are 107.48 (12) and 103.82 (9)°, respectively. These bond lengths and angles are all in the normal ranges and compare well those observed in other analogues (Allen *et al.*, 1987; Casabo *et al.*, 1995).

Experimental

The title compound was prepared according to the literature method of Mikhailov *et al.* (1984). 9,10-Bis(chloromethyl)anthracene (Miller *et al.*, 1955) (2.75 g, 0.01 mol) was added to a hot solution (about 323 K) of thiophenol sodium salt (2.64 g, 0.02 mol) in ethanol (30 ml), and the mixture was further stirred at 323 K for 6 h. After cooling, water (30 ml) was added and the resulting mixture left to stand for 5 h. The yellow precipitate was filtered off, washed with ethanol and water, and recrystallized from a mixture of chloroform and methanol, giving single crystals suitable for X-ray diffraction (yield 3.17 g, 75%, m.p. 518–520 K). Analysis calculated for $C_{28}H_{22}S_2$: C 79.58, H 5.25, S 15.17%; found: C 79.23, H 5.04, S 14.92%.

Crystal data

$C_{28}H_{22}S_2$
$M_r = 422.58$
Monoclinic, $P2_1/n$
$a = 7.318$ (2) Å
$b = 9.736$ (3) Å
$c = 15.433$ (5) Å
$\beta = 98.178$ (5)°
$V = 1088.3$ (6) Å^3
$Z = 2$
$D_x = 1.290$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 897 reflections
$\theta = 2.5$–24.3°
$\mu = 0.26$ mm^{-1}
$T = 293$ (2) K
Block, yellow
0.22 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detecter diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.946$, $T_{max} = 0.955$
6070 measured reflections
2215 independent reflections
1536 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 26.4°$
$h = -8 \rightarrow 9$
$k = -11 \rightarrow 12$
$l = -19 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.100$
$S = 1.02$
2215 reflections
136 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0452P)^2 + 0.1025P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}

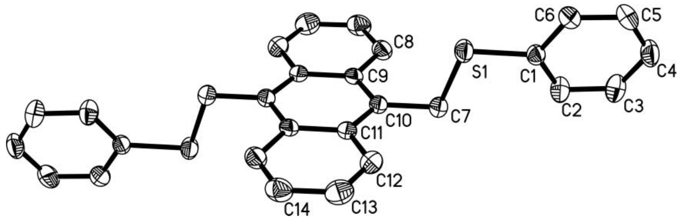


Figure 1
A drawing of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Unlabelled atoms are related by the symmetry code $(1 - x, 2 - y, 1 - z)$.

The H atoms were positioned geometrically and refined using a riding model, with fixed C—H distances of 0.93 (CH) and 0.96 Å (CH_2) [$U_{iso}(H) = 1.2U_{eq}(C)$].

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1997); software used to prepare material for publication: *SHELXTL*.

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