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1,4-Bis(methylsulfanyl)naphthalene

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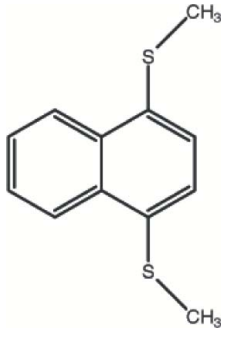
Key indicators: single-crystal synchrotron study; T = 153 K; mean σ(C–C) = 0.002 Å; R factor = 0.036; wR factor = 0.109; data-to-parameter ratio = 23.7.

The molecule of the title compound, $C_{12}H_{12}S_2$, is close to planar, with the methyl C atoms deviating by 0.019 (1) and 0.221 (2) Å from the naphthalene mean plane. In the crystal structure, the shortest S···S contact of 3.6864 (9) Å is longer than the van der Waals contact distance.

Related literature

For general background, see: Underhill (1992); Öncü *et al.* (2006). For related structures, see: Noreland *et al.* (1992, 1993). For bond-length data, see: Allen *et al.* (1987). For van der Waals radii, see: Bondi (1964).



Experimental

Crystal data

$C_{12}H_{12}S_2$ M_r = 220.34
Monoclinic, $P2_1/c$
a = 15.203 (3) Å
b = 10.246 (2) Å
c = 7.1750 (14) Å
β = 99.43 (3)°
V = 1102.6 (4) Å^3
Z = 4
Synchrotron radiation
λ = 0.75140 Å
μ = 0.44 mm^{-1}
T = 153 K
0.11 × 0.08 × 0.02 mm

Data collection

Bruker $P4$ diffractometer
Absorption correction: part of the refinement model (ΔF) (*XABS2*; Parkin *et al.*, 1995)
T_{min} = 0.832, T_{max} = 0.991
5197 measured reflections
3013 independent reflections
2619 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.109
S = 1.07
3013 reflections
127 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Data collection: *XSCANS* (Bruker, 1996); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: direct methods using *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2962).

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S1. Comment

Molecular electronics have attracted considerable attention because they are used for production electronic switches, memory cells or sensors. The most extensive range of the set compounds is based on planar organic donor molecules containing S or Se atoms (*e.g.* Underhill, 1992; Noreland *et al.*, 1992; Noreland *et al.*, 1993; Öncü *et al.*, 2006. In this study, the synthesis and structure of the title compound, (I), are reported.

As shown in Fig. 1, the naphthalene group (C1–C10) of the title molecule (I) is essentially planar, with maximum deviations of -0.014 (1), -0.014 (1) and 0.018 (1) Å for C4, C8 and C6, respectively. Deviations from planarity in the title molecule which were calculated to the least-squares plane of the naphthalene group are: 0.014 (1) Å for S1, 0.112 (1) Å for S2, -0.221 (2) Å for C11 and -0.019 (1) Å for C12. The bond lengths and angles in (I) show normal values (Allen *et al.*, 1987). The molecular packing of (I) as seen down the *a* axis is illustrated in Fig. 2. There is only one S···S contact near the van der Waals contact distance, 3.6 Å (Bondi, 1964): S2···S2^{i} 3.6864 (9) Å [symmetry code: (i) -*x* + 1, -*y*, -*z*].

S2. Experimental

The complete reaction was carried out under nitrogen atmosphere and 195 K. t-BuLi (10 ml, 14 mmol) solution was added to 1,4-dibromonaphthalene (1 g, 3.5 mmol) solved in dry THF (12 ml) with continuous stirring. Meanwhile, red colour was observed because of LiBr formation. Later, to the resulting reaction mixture was added dropwise $(CH_3S)_2$ (1.24 ml, 14 mmol). After 1 h, the reaction was ended. Reaction mixture warming to room temperature was extracted with Et_2O (3 × 25 ml). The extract was dried over Na_2SO_4 and concentrated. 1,4-Bis(methylthio)naphthalene as white needle-like crystals was obtained by crystallization from crude product solved in dichloromethane:hexan (1:19) system (708 mg, 92%), m.p. 369–371 K (lit. 370–371 K).

S3. Refinement

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic H atoms, and 0.9 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms.

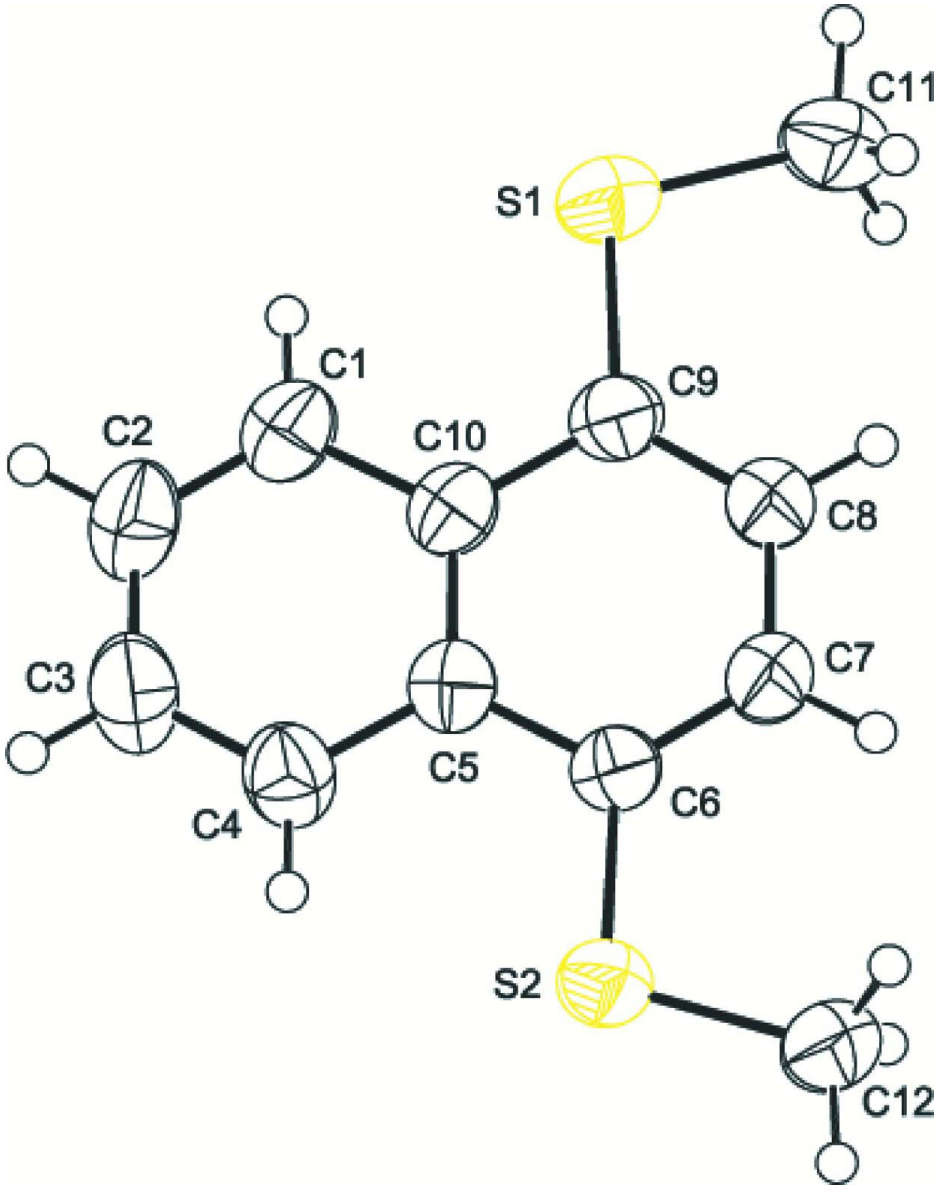

Figure 1

The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level.

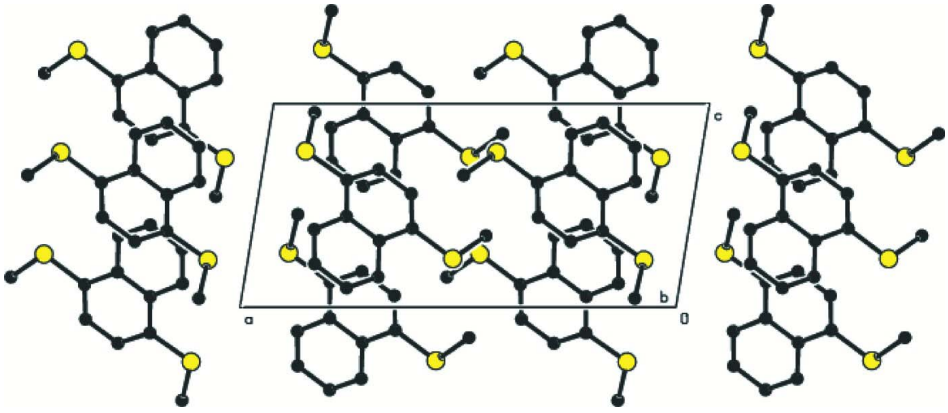

Figure 2

View of the molecular packing diagram of compound (I) viewed down *b* axis. H atoms have been omitted for clarity.

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Crystal data

$C_{12}H_{12}S_2$
$M_r = 220.34$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 15.203$ (3) Å
$b = 10.246$ (2) Å
$c = 7.1750$ (14) Å
$\beta = 99.43$ (3)°
$V = 1102.6$ (4) Å^3
$Z = 4$
$F(000) = 464$
$D_x = 1.327$ Mg m^{-3}
Synchrotron radiation, $\lambda = 0.75140$ Å
Cell parameters from 40396 reflections
$\theta = 1.0$–$27.0°$
$\mu = 0.44$ mm^{-1}
$T = 153$ K
Prism, colourless
0.11 × 0.08 × 0.02 mm

Data collection

Bruker P4 diffractometer
Radiation source: sealed tube
Graphite monochromator
ω scans
Absorption correction: part of the refinement model (ΔF) (*XABS2*; Parkin *et al.*, 1995)
$T_{min} = 0.832$, $T_{max} = 0.991$
5197 measured reflections
3013 independent reflections
2619 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$
$\theta_{max} = 33.8°$, $\theta_{min} = 2.6°$
$h = -20 \rightarrow 20$
$k = -14 \rightarrow 14$
$l = -9 \rightarrow 0$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.109$
$S = 1.07$
3013 reflections
127 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\Sigma^2(F_o^2) + (0.0553P)^2 + 0.1466P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

Special details

Experimental. Cubic fit to sin(theta)/lambda - 24 parameters

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.90863 (2)	−0.04680 (4)	0.76728 (6)	0.0671 (2)
S2	0.53023 (2)	−0.06992 (3)	0.23860 (5)	0.0558 (1)
C1	0.85913 (9)	0.07840 (13)	0.3828 (2)	0.0578 (4)
C2	0.84525 (11)	0.14096 (16)	0.2131 (2)	0.0700 (5)
C3	0.76299 (11)	0.13355 (17)	0.0952 (2)	0.0714 (5)
C4	0.69472 (10)	0.06351 (14)	0.1496 (2)	0.0592 (4)
C5	0.70573 (8)	−0.00085 (11)	0.32680 (17)	0.0468 (3)
C6	0.63478 (8)	−0.07293 (11)	0.38797 (18)	0.0469 (3)
C7	0.65018 (9)	−0.13631 (14)	0.55763 (19)	0.0562 (4)
C8	0.73388 (9)	−0.13004 (14)	0.67599 (19)	0.0585 (4)
C9	0.80296 (8)	−0.05983 (12)	0.62517 (19)	0.0511 (4)
C10	0.79008 (8)	0.00626 (11)	0.44685 (18)	0.0478 (3)
C11	0.90238 (12)	−0.15800 (18)	0.9562 (3)	0.0818 (6)
C12	0.46292 (9)	−0.17829 (14)	0.3515 (2)	0.0625 (4)
H1	0.91490	0.08300	0.45830	0.0690*
H2	0.89120	0.18910	0.17560	0.0840*
H3	0.75440	0.17620	−0.02070	0.0860*
H4	0.64030	0.05810	0.06910	0.0710*
H7	0.60450	−0.18460	0.59600	0.0670*
H8	0.74230	−0.17440	0.79060	0.0700*
H11A	0.95780	−0.15720	1.04240	0.1230*
H11B	0.89100	−0.24440	0.90620	0.1230*
H11C	0.85490	−0.13220	1.02170	0.1230*
H12A	0.40410	−0.18270	0.27870	0.0940*
H12B	0.45940	−0.14650	0.47600	0.0940*
H12C	0.48920	−0.26370	0.36040	0.0940*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0534 (2)	0.0744 (3)	0.0682 (3)	−0.0142 (2)	−0.0060 (2)	0.0043 (2)
S2	0.0519 (2)	0.0567 (2)	0.0553 (2)	−0.0028 (1)	−0.0020 (1)	0.0051 (1)
C1	0.0503 (7)	0.0558 (7)	0.0691 (8)	−0.0030 (5)	0.0149 (6)	0.0008 (6)
C2	0.0643 (8)	0.0693 (9)	0.0818 (10)	−0.0055 (7)	0.0280 (7)	0.0134 (7)
C3	0.0707 (9)	0.0773 (10)	0.0696 (9)	0.0035 (7)	0.0212 (7)	0.0236 (8)

C4	0.0578 (7)	0.0612 (7)	0.0593 (8)	0.0062 (5)	0.0117 (6)	0.0111 (6)
C5	0.0494 (6)	0.0417 (5)	0.0504 (6)	0.0037 (4)	0.0116 (4)	0.0001 (4)
C6	0.0453 (6)	0.0447 (5)	0.0497 (6)	0.0001 (4)	0.0047 (4)	−0.0012 (4)
C7	0.0490 (6)	0.0610 (7)	0.0571 (7)	−0.0094 (5)	0.0043 (5)	0.0098 (6)
C8	0.0540 (7)	0.0660 (8)	0.0528 (7)	−0.0088 (6)	0.0007 (5)	0.0117 (6)
C9	0.0473 (6)	0.0505 (6)	0.0537 (7)	−0.0036 (5)	0.0031 (5)	−0.0019 (5)
C10	0.0484 (6)	0.0411 (5)	0.0550 (6)	0.0002 (4)	0.0115 (5)	−0.0026 (5)
C11	0.0770 (10)	0.0848 (11)	0.0728 (10)	−0.0151 (9)	−0.0198 (8)	0.0164 (8)
C12	0.0536 (7)	0.0643 (8)	0.0667 (8)	−0.0097 (6)	0.0017 (6)	0.0023 (6)

Geometric parameters (Å, º)

S1—C9	1.7611 (14)	C9—C10	1.4324 (18)
S1—C11	1.785 (2)	C1—H1	0.9300
S2—C6	1.7657 (13)	C2—H2	0.9300
S2—C12	1.7911 (15)	C3—H3	0.9300
C1—C2	1.362 (2)	C4—H4	0.9300
C1—C10	1.4204 (19)	C7—H7	0.9300
C2—C3	1.392 (2)	C8—H8	0.9300
C3—C4	1.370 (2)	C11—H11A	0.9600
C4—C5	1.4176 (19)	C11—H11B	0.9600
C5—C6	1.4341 (17)	C11—H11C	0.9600
C5—C10	1.4247 (18)	C12—H12A	0.9600
C6—C7	1.3656 (19)	C12—H12B	0.9600
C7—C8	1.411 (2)	C12—H12C	0.9600
C8—C9	1.3707 (19)		
S2···S2^{i}	3.6864 (9)		
C9—S1—C11	103.55 (8)	C1—C2—H2	120.00
C6—S2—C12	103.82 (7)	C3—C2—H2	120.00
C2—C1—C10	121.32 (14)	C2—C3—H3	120.00
C1—C2—C3	120.65 (15)	C4—C3—H3	120.00
C2—C3—C4	120.16 (14)	C3—C4—H4	120.00
C3—C4—C5	121.03 (14)	C5—C4—H4	119.00
C4—C5—C6	121.99 (12)	C6—C7—H7	119.00
C4—C5—C10	118.74 (12)	C8—C7—H7	119.00
C6—C5—C10	119.27 (11)	C7—C8—H8	119.00
S2—C6—C5	116.91 (10)	C9—C8—H8	119.00
S2—C6—C7	123.72 (10)	S1—C11—H11A	109.00
C5—C6—C7	119.34 (12)	S1—C11—H11B	109.00
C6—C7—C8	121.39 (13)	S1—C11—H11C	109.00
C7—C8—C9	121.24 (13)	H11A—C11—H11B	110.00
S1—C9—C8	123.49 (11)	H11A—C11—H11C	109.00
S1—C9—C10	117.36 (10)	H11B—C11—H11C	109.00
C8—C9—C10	119.15 (12)	S2—C12—H12A	109.00
C1—C10—C5	118.08 (12)	S2—C12—H12B	109.00
C1—C10—C9	122.34 (12)	S2—C12—H12C	109.00

C5—C10—C9	119.58 (11)	H12A—C12—H12B	109.00
C2—C1—H1	119.00	H12A—C12—H12C	109.00
C10—C1—H1	119.00	H12B—C12—H12C	109.00
C11—S1—C9—C8	7.08 (14)	C10—C5—C6—C7	−1.81 (18)
C11—S1—C9—C10	−172.38 (11)	C4—C5—C10—C1	0.28 (18)
C12—S2—C6—C5	175.91 (10)	C4—C5—C10—C9	−179.02 (12)
C12—S2—C6—C7	−5.94 (13)	C6—C5—C10—C1	−179.94 (12)
C10—C1—C2—C3	−1.4 (2)	C6—C5—C10—C9	0.76 (17)
C2—C1—C10—C5	1.0 (2)	S2—C6—C7—C8	−176.70 (11)
C2—C1—C10—C9	−179.70 (14)	C5—C6—C7—C8	1.4 (2)
C1—C2—C3—C4	0.4 (2)	C6—C7—C8—C9	0.1 (2)
C2—C3—C4—C5	0.9 (2)	C7—C8—C9—S1	179.38 (11)
C3—C4—C5—C6	178.97 (14)	C7—C8—C9—C10	−1.2 (2)
C3—C4—C5—C10	−1.3 (2)	S1—C9—C10—C1	0.93 (17)
C4—C5—C6—S2	−3.80 (16)	S1—C9—C10—C5	−179.80 (10)
C4—C5—C6—C7	177.96 (13)	C8—C9—C10—C1	−178.56 (13)
C10—C5—C6—S2	176.43 (9)	C8—C9—C10—C5	0.71 (18)

Symmetry code: (i) −*x*+1, −*y*, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···S1	0.93	2.60	3.0235 (16)	108
C4—H4···S2	0.93	2.58	3.0090 (17)	108