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1-Bromo-8-(ethylsulfanyl)naphthalene

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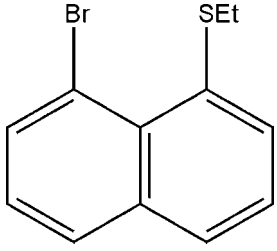
Key indicators: single-crystal X-ray study; T = 125 K; mean σ(C–C) = 0.009 Å; R factor = 0.053; wR factor = 0.106; data-to-parameter ratio = 13.9.

There are two molecules in the asymmetric unit of the title compound, $C_{12}H_{11}BrS$, with similar conformations. Intramolecular Br···S(ethyl) distances are 3.056 (2) and 3.050 (2) Å. The molecules pack into a herringbone array with no significant π–π interactions.

Related literature

For background, see: Aucott *et al.* (2004). For synthesis, see Oki & Yamada (1988).



Experimental

Crystal data

$C_{12}H_{11}BrS$
M_r = 267.18
Monoclinic, $P2_1/c$
a = 11.632 (4) Å
b = 12.260 (4) Å
c = 14.748 (4) Å
β = 91.692 (9)°
V = 2102.2 (11) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 4.06 mm^{-1}
T = 125 (2) K
0.25 × 0.20 × 0.20 mm

Data collection

Rigaku SCXmini CCD diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.396, T_{max} = 0.452
6713 measured reflections
3543 independent reflections
2316 reflections with $I > 2\sigma(I)$
R_{int} = 0.079

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.106
S = 0.99
3543 reflections
254 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C22—H22A···Br1	0.95	3.025	3.957 (2)	167

Data collection: *SCXmini* (Rigaku, 2006); cell refinement: *PROCESS-AUTO* (Rigaku, 1998); data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CrystalStructure* (Rigaku, 2006); software used to prepare material for publication: *CrystalStructure*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2511).

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supplementary materials

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1-Bromo-8-(ethylsulfanyl)naphthalene

A. L. Fuller, F. R. Knight, A. M. Z. Slawin and J. D. Woollins

Comment

As part of a broader study into sterically crowded naphthalene derivatives (Aucott *et al.*, 2004), here we report the structure of the title compound, (I), (Fig. 1), which contains two independent molecules. The intramolecular Br···SEt distances are 3.056 (2) and 3.050 (2) Å. The bromine and sulfur atoms show minor deviations above/below their attached ring planes: S9 = 0.022 (2) Å, S29 = −0.016 (2) Å, Br1 = −0.117 (1) Å and Br21 = −0.018 (1) Å. naphthalene planes

The molecules pack in a herringbone array with no significant π–π interactions. The shortest intermolecular S···S distance is 4.199 (2) Å and there is a weak intermolecular C—H···Br interaction [for C22–H22A···Br1: H···Br = 3.025 Å, C—H···Br = 167°].

Experimental

The title compound was prepared as described previously (Oki & Yamada, 1988) and colourless blocks of (I) were recystallized from n-hexane.

Refinement

All the H atoms were geometrically placed (C—H = 0.95–0.97 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

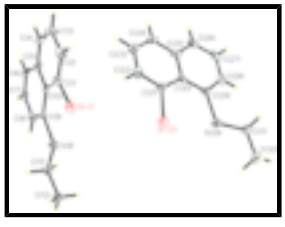


Fig. 1. The molecular structure of (I) with displacement ellipsoids drawn at the 50% probability level (arbitrary spheres for the H atoms).

1-Bromo-8-(ethylsulfanyl)naphthalene

Crystal data

$C_{12}H_{11}BrS$	F_{000} = 1072
M_r = 267.18	D_x = 1.688 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3763 reflections

a = 11.632 (4) Å	θ = 1.6–25.2º
b = 12.260 (4) Å	μ = 4.06 mm^{-1}
c = 14.748 (4) Å	T = 125 (2) K
β = 91.692 (9)º	Block, colourless
V = 2102.2 (11) $Å^3$	0.25 × 0.20 × 0.20 mm
Z = 8	

Data collection

Rigaku SCXmini CCD diffractometer	3543 independent reflections
Radiation source: fine-focus sealed tube	2316 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.079
T = 125(2) K	θ_{max} = 25.0º
ω scans	θ_{min} = 7.8º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	h = 0→13
T_{min} = 0.396, T_{max} = 0.452	k = −14→14
6713 measured reflections	l = −17→17

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.053	H-atom parameters constrained
$wR(F^2)$ = 0.106	$w = 1/[\sigma^2(F_o^2) + (0.044P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.99	$(\Delta/\sigma)_{max} < 0.001$
3543 reflections	$\Delta\rho_{max}$ = 0.46 e $Å^{-3}$
254 parameters	$\Delta\rho_{min}$ = −0.47 e $Å^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness 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 threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating *R*-factors(gt) *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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.07289 (6)	0.47998 (5)	0.38936 (4)	0.02453 (19)
C1	0.0346 (5)	0.4500 (5)	0.2657 (4)	0.0190 (14)
C2	−0.0539 (6)	0.5134 (6)	0.2332 (4)	0.0275 (15)
H2A	−0.0850	0.5682	0.2709	0.033*
C3	−0.0995 (6)	0.4985 (6)	0.1450 (5)	0.0291 (17)
H3A	−0.1620	0.5418	0.1229	0.035*
C4	−0.0529 (5)	0.4216 (6)	0.0921 (4)	0.0229 (15)
H4A	−0.0837	0.4111	0.0323	0.027*
C5	0.0391 (5)	0.3568 (5)	0.1223 (4)	0.0201 (14)
C6	0.0854 (5)	0.2758 (5)	0.0626 (4)	0.0191 (14)
H6A	0.0515	0.2656	0.0038	0.023*
C7	0.1740 (6)	0.2160 (5)	0.0887 (4)	0.0195 (14)
H7A	0.2043	0.1642	0.0478	0.023*
C8	0.2248 (6)	0.2269 (5)	0.1753 (4)	0.0222 (14)
H8A	0.2887	0.1821	0.1917	0.027*
C9	0.1853 (5)	0.3003 (5)	0.2373 (4)	0.0172 (13)
C10	0.0884 (5)	0.3688 (5)	0.2130 (3)	0.0138 (12)
S9	0.25526 (14)	0.31016 (13)	0.34520 (10)	0.0209 (4)
C11	0.3730 (6)	0.2139 (5)	0.3396 (4)	0.0222 (14)
H11A	0.3434	0.1385	0.3332	0.027*
H11B	0.4215	0.2304	0.2872	0.027*
C12	0.4421 (6)	0.2271 (5)	0.4288 (4)	0.0253 (15)
H12A	0.5073	0.1766	0.4298	0.038*
H12B	0.3926	0.2111	0.4798	0.038*
H12C	0.4705	0.3022	0.4339	0.038*
Br21	0.33155 (6)	0.74894 (6)	0.39260 (4)	0.0266 (2)
C21	0.2805 (5)	0.7861 (5)	0.2732 (4)	0.0184 (14)
C22	0.1837 (6)	0.7288 (5)	0.2451 (4)	0.0254 (15)
H22A	0.1494	0.6781	0.2848	0.031*
C23	0.1365 (6)	0.7454 (6)	0.1584 (4)	0.0270 (15)
H23A	0.0708	0.7048	0.1387	0.032*
C24	0.1827 (6)	0.8179 (5)	0.1030 (4)	0.0236 (15)
H24A	0.1493	0.8279	0.0440	0.028*
C25	0.2803 (5)	0.8805 (5)	0.1297 (4)	0.0209 (14)
C26	0.3233 (6)	0.9574 (5)	0.0688 (4)	0.0220 (15)
H26A	0.2874	0.9659	0.0106	0.026*
C27	0.4170 (6)	1.0206 (6)	0.0931 (4)	0.0261 (15)
H27A	0.4446	1.0742	0.0525	0.031*
C28	0.4710 (6)	1.0053 (5)	0.1774 (4)	0.0255 (15)
H28A	0.5368	1.0481	0.1929	0.031*
C29	0.4327 (5)	0.9304 (5)	0.2397 (4)	0.0186 (13)
C30	0.3345 (5)	0.8662 (5)	0.2180 (4)	0.0164 (13)
S29	0.50989 (14)	0.92059 (13)	0.34520 (10)	0.0221 (4)
C31	0.6292 (5)	1.0142 (5)	0.3351 (4)	0.0227 (14)
H31A	0.6778	0.9927	0.2841	0.027*

H31B	0.6008	1.0893	0.3243	0.027*
C32	0.6973 (6)	1.0079 (6)	0.4242 (5)	0.0309 (17)
H32A	0.7635	1.0571	0.4221	0.046*
H32B	0.7243	0.9330	0.4341	0.046*
H32C	0.6481	1.0295	0.4739	0.046*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0280 (4)	0.0259 (3)	0.0197 (3)	0.0037 (3)	−0.0004 (3)	−0.0061 (3)
C1	0.021 (3)	0.018 (3)	0.018 (3)	0.001 (3)	0.003 (3)	−0.002 (2)
C2	0.031 (4)	0.025 (4)	0.027 (3)	0.003 (3)	0.006 (3)	0.001 (3)
C3	0.019 (3)	0.045 (5)	0.024 (3)	0.010 (3)	−0.001 (3)	0.015 (3)
C4	0.013 (3)	0.039 (4)	0.016 (3)	−0.004 (3)	−0.002 (3)	0.004 (3)
C5	0.021 (3)	0.026 (3)	0.014 (3)	−0.009 (3)	0.002 (3)	0.001 (3)
C6	0.015 (3)	0.032 (4)	0.010 (3)	−0.010 (3)	−0.005 (2)	−0.001 (3)
C7	0.026 (4)	0.019 (3)	0.013 (3)	−0.009 (3)	0.003 (3)	−0.006 (2)
C8	0.025 (4)	0.018 (3)	0.024 (3)	0.001 (3)	0.003 (3)	0.004 (3)
C9	0.018 (3)	0.014 (3)	0.019 (3)	−0.004 (3)	−0.006 (3)	0.005 (3)
C10	0.013 (3)	0.022 (3)	0.006 (3)	−0.009 (3)	−0.001 (2)	0.003 (2)
S9	0.0258 (9)	0.0229 (8)	0.0140 (7)	0.0070 (7)	−0.0020 (7)	−0.0021 (6)
C11	0.025 (4)	0.022 (3)	0.019 (3)	0.004 (3)	−0.003 (3)	−0.001 (3)
C12	0.025 (4)	0.026 (4)	0.024 (3)	0.008 (3)	−0.008 (3)	0.002 (3)
Br21	0.0342 (4)	0.0279 (4)	0.0174 (3)	−0.0057 (3)	−0.0042 (3)	0.0074 (3)
C21	0.020 (3)	0.021 (3)	0.014 (3)	0.005 (3)	−0.001 (3)	−0.005 (2)
C22	0.025 (4)	0.024 (4)	0.028 (3)	−0.003 (3)	0.006 (3)	−0.003 (3)
C23	0.021 (4)	0.034 (4)	0.026 (4)	0.003 (3)	−0.004 (3)	−0.010 (3)
C24	0.021 (4)	0.034 (4)	0.015 (3)	0.012 (3)	−0.004 (3)	−0.004 (3)
C25	0.021 (3)	0.028 (4)	0.013 (3)	0.016 (3)	0.000 (3)	−0.006 (3)
C26	0.027 (4)	0.027 (4)	0.012 (3)	0.012 (3)	0.002 (3)	0.002 (3)
C27	0.035 (4)	0.024 (3)	0.020 (3)	0.007 (3)	0.014 (3)	0.012 (3)
C28	0.032 (4)	0.015 (3)	0.029 (3)	−0.004 (3)	0.005 (3)	−0.003 (3)
C29	0.019 (3)	0.021 (3)	0.016 (3)	0.008 (3)	0.001 (3)	−0.001 (3)
C30	0.023 (3)	0.013 (3)	0.014 (3)	0.008 (3)	0.001 (2)	−0.005 (2)
S29	0.0246 (9)	0.0236 (9)	0.0179 (8)	−0.0030 (7)	−0.0032 (7)	0.0010 (7)
C31	0.021 (3)	0.022 (3)	0.025 (3)	−0.001 (3)	−0.003 (3)	−0.002 (3)
C32	0.031 (4)	0.027 (4)	0.034 (4)	−0.008 (3)	−0.007 (3)	−0.004 (3)

Geometric parameters (Å, °)

Br1—C1	1.901 (6)	Br21—C21	1.897 (6)
C1—C2	1.365 (9)	C21—C22	1.381 (9)
C1—C10	1.419 (8)	C21—C30	1.433 (9)
C2—C3	1.403 (10)	C22—C23	1.391 (9)
C2—H2A	0.9500	C22—H22A	0.9500
C3—C4	1.348 (9)	C23—C24	1.331 (10)
C3—H3A	0.9500	C23—H23A	0.9500
C4—C5	1.395 (9)	C24—C25	1.417 (10)
C4—H4A	0.9500	C24—H24A	0.9500

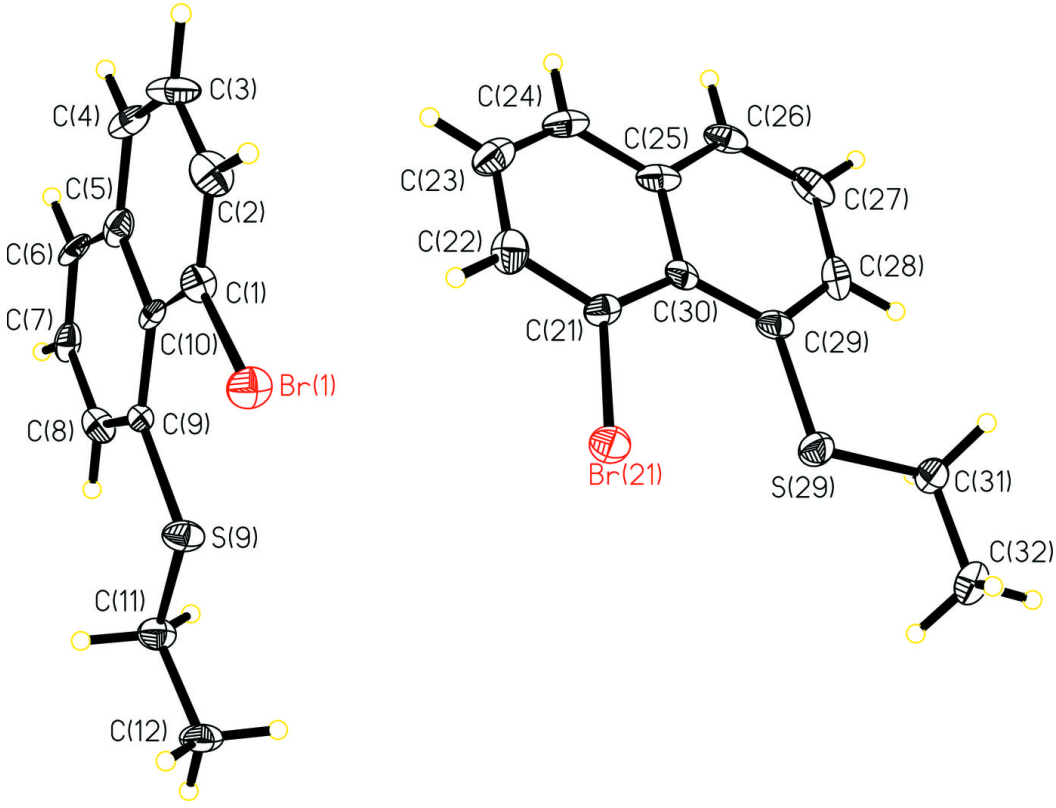
C5—C6	1.443 (9)	C25—C26	1.404 (9)
C5—C10	1.446 (8)	C25—C30	1.441 (8)
C6—C7	1.312 (9)	C26—C27	1.376 (10)
C6—H6A	0.9500	C26—H26A	0.9500
C7—C8	1.398 (8)	C27—C28	1.388 (10)
C7—H7A	0.9500	C27—H27A	0.9500
C8—C9	1.371 (9)	C28—C29	1.382 (9)
C8—H8A	0.9500	C28—H28A	0.9500
C9—C10	1.443 (8)	C29—C30	1.415 (9)
C9—S9	1.770 (6)	C29—S29	1.778 (6)
S9—C11	1.811 (7)	S29—C31	1.810 (7)
C11—C12	1.530 (9)	C31—C32	1.516 (9)
C11—H11A	0.9900	C31—H31A	0.9900
C11—H11B	0.9900	C31—H31B	0.9900
C12—H12A	0.9800	C32—H32A	0.9800
C12—H12B	0.9800	C32—H32B	0.9800
C12—H12C	0.9800	C32—H32C	0.9800
C2—C1—C10	123.2 (6)	C22—C21—C30	123.1 (5)
C2—C1—Br1	112.3 (5)	C22—C21—Br21	112.8 (5)
C10—C1—Br1	124.5 (4)	C30—C21—Br21	124.1 (4)
C1—C2—C3	120.8 (6)	C21—C22—C23	119.9 (6)
C1—C2—H2A	119.6	C21—C22—H22A	120.1
C3—C2—H2A	119.6	C23—C22—H22A	120.1
C4—C3—C2	118.7 (6)	C24—C23—C22	120.4 (6)
C4—C3—H3A	120.6	C24—C23—H23A	119.8
C2—C3—H3A	120.6	C22—C23—H23A	119.8
C3—C4—C5	122.0 (6)	C23—C24—C25	121.7 (6)
C3—C4—H4A	119.0	C23—C24—H24A	119.1
C5—C4—H4A	119.0	C25—C24—H24A	119.1
C4—C5—C6	119.5 (5)	C26—C25—C24	118.9 (5)
C4—C5—C10	121.1 (6)	C26—C25—C30	120.3 (6)
C6—C5—C10	119.3 (6)	C24—C25—C30	120.8 (6)
C7—C6—C5	120.6 (5)	C27—C26—C25	120.4 (5)
C7—C6—H6A	119.7	C27—C26—H26A	119.8
C5—C6—H6A	119.7	C25—C26—H26A	119.8
C6—C7—C8	121.5 (6)	C26—C27—C28	119.4 (6)
C6—C7—H7A	119.3	C26—C27—H27A	120.3
C8—C7—H7A	119.3	C28—C27—H27A	120.3
C9—C8—C7	122.1 (6)	C29—C28—C27	122.6 (6)
C9—C8—H8A	119.0	C29—C28—H28A	118.7
C7—C8—H8A	119.0	C27—C28—H28A	118.7
C8—C9—C10	119.4 (5)	C28—C29—C30	119.6 (6)
C8—C9—S9	119.4 (5)	C28—C29—S29	117.5 (5)
C10—C9—S9	121.2 (4)	C30—C29—S29	122.9 (5)
C1—C10—C9	128.8 (5)	C29—C30—C21	128.1 (5)
C1—C10—C5	114.1 (5)	C29—C30—C25	117.7 (6)
C9—C10—C5	117.1 (5)	C21—C30—C25	114.1 (5)
C9—S9—C11	104.0 (3)	C29—S29—C31	104.7 (3)
C12—C11—S9	105.7 (4)	C32—C31—S29	106.2 (5)

C12—C11—H11A	110.6	C32—C31—H31A	110.5
S9—C11—H11A	110.6	S29—C31—H31A	110.5
C12—C11—H11B	110.6	C32—C31—H31B	110.5
S9—C11—H11B	110.6	S29—C31—H31B	110.5
H11A—C11—H11B	108.7	H31A—C31—H31B	108.7
C11—C12—H12A	109.5	C31—C32—H32A	109.5
C11—C12—H12B	109.5	C31—C32—H32B	109.5
H12A—C12—H12B	109.5	H32A—C32—H32B	109.5
C11—C12—H12C	109.5	C31—C32—H32C	109.5
H12A—C12—H12C	109.5	H32A—C32—H32C	109.5
H12B—C12—H12C	109.5	H32B—C32—H32C	109.5
C10—C1—C2—C3	2.1 (10)	C30—C21—C22—C23	2.1 (9)
Br1—C1—C2—C3	−175.9 (5)	Br21—C21—C22—C23	−179.0 (5)
C1—C2—C3—C4	−1.1 (10)	C21—C22—C23—C24	−1.4 (9)
C2—C3—C4—C5	−0.2 (10)	C22—C23—C24—C25	−0.2 (10)
C3—C4—C5—C6	−180.0 (6)	C23—C24—C25—C26	−178.5 (6)
C3—C4—C5—C10	0.6 (10)	C23—C24—C25—C30	1.2 (9)
C4—C5—C6—C7	178.1 (6)	C24—C25—C26—C27	179.1 (6)
C10—C5—C6—C7	−2.5 (9)	C30—C25—C26—C27	−0.6 (9)
C5—C6—C7—C8	1.4 (9)	C25—C26—C27—C28	1.9 (9)
C6—C7—C8—C9	−0.1 (9)	C26—C27—C28—C29	−1.6 (10)
C7—C8—C9—C10	0.0 (9)	C27—C28—C29—C30	−0.2 (9)
C7—C8—C9—S9	−179.4 (5)	C27—C28—C29—S29	−179.6 (5)
C2—C1—C10—C9	176.8 (6)	C28—C29—C30—C21	−178.9 (6)
Br1—C1—C10—C9	−5.5 (9)	S29—C29—C30—C21	0.4 (9)
C2—C1—C10—C5	−1.5 (9)	C28—C29—C30—C25	1.6 (8)
Br1—C1—C10—C5	176.2 (4)	S29—C29—C30—C25	−179.2 (4)
C8—C9—C10—C1	−179.4 (6)	C22—C21—C30—C29	179.3 (6)
S9—C9—C10—C1	−0.1 (9)	Br21—C21—C30—C29	0.5 (9)
C8—C9—C10—C5	−1.0 (8)	C22—C21—C30—C25	−1.1 (8)
S9—C9—C10—C5	178.3 (4)	Br21—C21—C30—C25	−179.9 (4)
C4—C5—C10—C1	0.2 (8)	C26—C25—C30—C29	−1.2 (8)
C6—C5—C10—C1	−179.2 (5)	C24—C25—C30—C29	179.1 (5)
C4—C5—C10—C9	−178.4 (6)	C26—C25—C30—C21	179.2 (5)
C6—C5—C10—C9	2.2 (8)	C24—C25—C30—C21	−0.5 (8)
C8—C9—S9—C11	2.1 (6)	C28—C29—S29—C31	−3.3 (6)
C10—C9—S9—C11	−177.2 (5)	C30—C29—S29—C31	177.4 (5)
C9—S9—C11—C12	175.2 (4)	C29—S29—C31—C32	−179.9 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C22—H22A···Br1	0.95	3.03	Missing	167

Fig. 1


C(3)
C(4)
C(5)
C(2)
C(6)
C(1)
C(7)
C(10)
Br(1)
C(8)
C(9)
S(9)
C(11)
C(12)
C(24)
C(25)
C(26)
C(23)
C(27)
C(22)
C(28)
C(21)
C(30)
C(29)
Br(21)
S(29)
C(31)
C(32)