Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

7-Bromo-2-methyl-1-(phenylsulfanyl)-naphtho[2,1-*b*]furan

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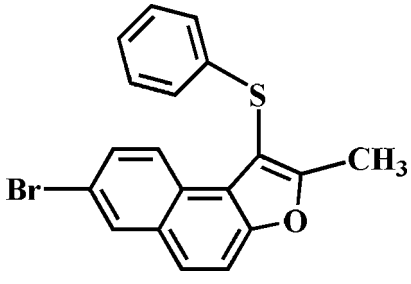
Received 12 September 2007; accepted 17 September 2007

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.009 Å; R factor = 0.058; wR factor = 0.152; data-to-parameter ratio = 13.1.

The title compound, $C_{19}H_{13}BrOS$, was prepared by the Lewis acid-catalyzed reaction of 6-bromo-2-naphthol and α-chloro-α-(phenylsulfanyl)acetone. There are two symmetry-independent molecules in the asymmetric unit. The phenyl rings are nearly perpendicular to the naphthofuran systems, with dihedral angles of 72.9 (1) and 80.5 (1)°. The crystal structure is stabilized by π–π stacking interactions between the brominated benzene ring and the furan fragment of the naphthofuran system from two symmetry-independent molecules; the centroid-to-centroid distances within the stack are 3.594 (9) and 3.658 (9) Å. Additionally, the stacked molecules exhibit short C—H$\cdots\pi$ contacts between the methyl H atoms and the central benzene ring of the naphthofuran system.

Related literature

For the crystal structures of similar naphthofuran compounds, see: Choi *et al.* (2006, 2007).



Experimental

Crystal data

$C_{19}H_{13}BrOS$
M_r = 369.26
Triclinic, $P\overline{1}$
a = 10.947 (2) Å
b = 11.130 (2) Å
c = 13.636 (2) Å
α = 112.798 (2)°
β = 91.999 (3)°
γ = 90.908 (2)°
V = 1529.9 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.82 mm^{-1}
T = 173 (2) K
0.35 × 0.25 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1999)
T_{min} = 0.442, T_{max} = 0.760
7613 measured reflections
5209 independent reflections
4269 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.152
S = 1.14
5209 reflections
398 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.65 e Å^{-3}

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

*Cg*3 and *Cg*5 are the centroids of the C21/C22/C27–C30 and C2/C3/C8–C11 benzene rings, respectively.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C19—H19*C*$\cdots$*Cg*3	0.98	2.77	3.551 (6)	137
C38—H38*A*$\cdots$*Cg*5	0.98	2.60	3.498 (6)	153

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2104).

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  doi:10.1107/S160053680704562X

supplementary materials

Acta Cryst. (2007). E**63**, o4102 [**doi:10.1107/S160053680704562X**]

7-Bromo-2-methyl-1-(phenylsulfanyl)naphtho[2,1-*b*]furan

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Comment

As part of our ongoing studies on the synthesis and structure of 2-methylnaphtho[2,1-*b*]furan analogues, we have recently described the crystal structures of 2-methyl-1-(methylsulfinyl)naphtho[2,1-*b*]furan (Choi *et al.*, 2006) and 2-methyl-1-(phenylsulfinyl)naphtho[2,1-*b*]furan (Choi *et al.*, 2007). Herein we report the molecular and crystal structure of the title compound, (Fig. 1).

The phenyl rings (C13—C18 in unit A and C32—C37 in unit B) are tilted towards the plane of the naphthofuran systems [72.9 (9)° (unit A) and 80.5 (1)° (unit B)]. The molecular packing (Fig. 2) is stabilized by two different π···π interactions within each stack of molecules; one between the benzene ring (*Cg*4) and an adjacent furan ring (*Cg*1) of benzofuran unit {distance; 3.594 (9) Å}, and a second between the benzene ring (*Cg*6) and an adjacent furan ring (*Cg*2) of benzofuran unit {distance; 3.658 (9) Å} (*Cg*1, *Cg*2, *Cg*4, and *Cg*6 are the centroids of the O1/C12/C1/C2/C11 furan ring, the O2/C31/C20/C21/C30 furan ring, the C22—C27 benzene ring, and the C3—C8 benzene ring, respectively; symmetry code as in Fig. 2). The crystal packing (Fig. 2) is further stabilized by CH_2—H···π interactions; one between the methyl group (unit B) and the benzene ring (unit A) of benzofuran unit, with a C38—H38A···*Cg*5 separation of 2.60 Å, and a second between the methyl group (Unit A) and the benzene ring (Unit B) of benzofuran unit, with a C19—H19C···*Cg*3 separation of 2.77 Å (Fig. 2 and Table 1; *Cg*3 and *Cg*5 are the centroids of the C21/C22/C27/C28/C29/C30 benzene ring and the C2/C3/C8/C9/C10/C11 benzene ring, respectively; symmetry code as in Fig. 2). In addition, the crystal packing (Fig. 2) is further stabilized by weak C—Br···π interactions: one between the Br atom (Unit B) and the phenyl ring (Unit A) with a C25—Br2···*Cg*8 separation of 3.718 (6) Å, and a second between the Br atom (Unit A) and the phenyl ring (Unit B) with a C6—Br1···*Cg*7 separation of 4.015 (6) Å (Fig. 2; *Cg*7 and *Cg*8 are the centroids of the C32—C37 benzene ring and the C13—C18 benzene ring, respectively; symmetry code as in Fig. 2).

Experimental

Zinc chloride (273 mg, 2.0 mmol) was added at room temperature to a stirred solution of 6-bromo-2-naphthol (446 mg, 2.0 mmol) and α-chloro-α-(phenylsulfanyl)acetone (401 mg, 2.0 mmol) in dichloromethane (30 ml), and stirred for 1 h. The mixture was quenched with water and the organic layer was separated, dried over magnesium sulfate, filtered and concentrated in vacuum. The residue was purified by column chromatography (CCl_4) to afford the title compound as a colorless solid [yield 63%, m.p. 436–437 K; R_f = 0.68 (CCl_4)]. Single crystals suitable for X-ray diffraction were prepared by slow evaporation of a dilute solution of the title compound in chloroform at room temperature.

Refinement

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.95 Å for aromatic H atoms and 0.98 Å for methyl H atoms, respectively, and with U_{iso}(H) = 1.2Ueq(C) for aromatic H atoms and U_{iso}(H) = 1.5Ueq(C) for methyl H atoms. The highest peak in the difference map is 1.13 Å from Br2 and the largest hole is 0.88 Å from Br1.

Figures

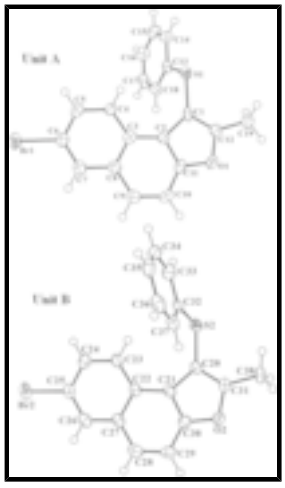


Fig. 1. The molecular structure of the title compound, showing displacement ellipsoides drawn at the 50% probability level.

Fig. 2. π···π, C—H···π and C—-Br···π intreactions (dotted lines) in the title compound. *Cg* denotes ring centroids. [Symmetry code: (i) *x*, 1 + *y*, *z*; (ii) −*x*, 1 − *y*, 2 − *z*; (iii) 1 − *x*, 1 − *y*, 2 − *z*.]

7-Bromo-2-methyl-1-(phenylsulfanyl)naphtho[2,1-*b*]furan

Crystal data

$C_{19}H_{13}BrOS$	$Z = 4$
$M_r = 369.26$	$F_{000} = 744$
Triclinic, $P\overline{1}$	$D_x = 1.603$ Mg m^{-3}
Hall symbol: -p 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 10.947$ (2) Å	Cell parameters from 4034 reflections
$b = 11.130$ (2) Å	$\theta = 2.4$–28.1º
$c = 13.636$ (2) Å	$\mu = 2.82$ mm^{-1}
$\alpha = 112.798$ (2)º	$T = 173$ (2) K
$\beta = 91.999$ (3)º	Plate, colorless
$\gamma = 90.908$ (2)º	0.35 × 0.25 × 0.10 mm
$V = 1529.9$ (5) Å^3	

Data collection

Bruker SMART CCD diffractometer	5209 independent reflections
Radiation source: fine-focus sealed tube	4269 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.025$
Detector resolution: 10.00 pixels mm^{-1}	$\theta_{max} = 25.0$º
$T = 173$(2) K	$\theta_{min} = 1.9$º
φ and ω scans	$h = -12 \rightarrow 13$

Absorption correction: multi-scan (SADABS; Sheldrick, 1999)

T_{min} = 0.442, T_{max} = 0.760

7613 measured reflections

k = −13→13

l = −6→16

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.058

$wR(F^2)$ = 0.152

S = 1.14

5209 reflections

398 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.0494P)^2 + 8.0396P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max}$ = 1.62 e Å^{-3}

$\Delta\rho_{min}$ = −0.65 e Å^{-3}

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	0.30246 (6)	0.23787 (6)	1.08462 (5)	0.0340 (2)
Br2	0.21489 (7)	0.73817 (6)	1.09288 (5)	0.0372 (2)
S1	−0.03179 (14)	0.56857 (14)	0.75823 (13)	0.0264 (3)
S2	0.49841 (14)	1.06833 (14)	0.75250 (13)	0.0271 (3)
O1	0.2948 (4)	0.5907 (4)	0.6588 (3)	0.0273 (9)
O2	0.1570 (4)	1.0853 (4)	0.6640 (3)	0.0286 (10)
C1	0.1213 (6)	0.5505 (5)	0.7258 (5)	0.0243 (13)
C2	0.2219 (5)	0.5038 (5)	0.7717 (5)	0.0232 (12)
C3	0.2368 (5)	0.4429 (5)	0.8456 (5)	0.0252 (13)
C4	0.1379 (5)	0.4037 (6)	0.8922 (5)	0.0267 (13)
H4	0.0565	0.4196	0.8750	0.032*
C5	0.1577 (6)	0.3435 (6)	0.9615 (5)	0.0304 (14)
H5	0.0906	0.3171	0.9917	0.036*
C6	0.2774 (6)	0.3212 (6)	0.9875 (5)	0.0276 (13)

C7	0.3755 (6)	0.3548 (6)	0.9445 (5)	0.0293 (14)
H7	0.4557	0.3370	0.9629	0.035*
C8	0.3579 (5)	0.4172 (6)	0.8714 (5)	0.0256 (13)
C9	0.4605 (6)	0.4532 (6)	0.8254 (5)	0.0288 (14)
H9	0.5407	0.4365	0.8446	0.035*
C10	0.4449 (6)	0.5118 (6)	0.7538 (5)	0.0316 (14)
H10	0.5126	0.5365	0.7232	0.038*
C11	0.3257 (6)	0.5329 (5)	0.7284 (5)	0.0253 (13)
C12	0.1696 (6)	0.5981 (6)	0.6569 (5)	0.0270 (13)
C13	−0.1025 (5)	0.4098 (6)	0.6961 (5)	0.0235 (12)
C14	−0.2286 (6)	0.4044 (6)	0.7031 (5)	0.0302 (14)
H14	−0.2712	0.4814	0.7403	0.036*
C15	−0.2910 (6)	0.2868 (7)	0.6559 (6)	0.0377 (16)
H15	−0.3772	0.2831	0.6607	0.045*
C16	−0.2308 (6)	0.1740 (6)	0.6014 (5)	0.0367 (16)
H16	−0.2749	0.0931	0.5689	0.044*
C17	−0.1065 (7)	0.1805 (6)	0.5950 (5)	0.0353 (16)
H17	−0.0646	0.1032	0.5568	0.042*
C18	−0.0398 (6)	0.2987 (6)	0.6434 (5)	0.0319 (15)
H18	0.0467	0.3020	0.6399	0.038*
C19	0.1166 (6)	0.6575 (6)	0.5860 (5)	0.0348 (15)
H19A	0.0272	0.6497	0.5844	0.052*
H19B	0.1454	0.6124	0.5140	0.052*
H19C	0.1421	0.7498	0.6127	0.052*
C20	0.3396 (5)	1.0475 (5)	0.7246 (5)	0.0228 (12)
C21	0.2475 (5)	0.9976 (5)	0.7729 (5)	0.0254 (13)
C22	0.2450 (5)	0.9334 (5)	0.8445 (5)	0.0242 (13)
C23	0.3499 (6)	0.8997 (6)	0.8901 (5)	0.0300 (14)
H23	0.4284	0.9178	0.8705	0.036*
C24	0.3419 (6)	0.8417 (6)	0.9618 (5)	0.0314 (14)
H24	0.4137	0.8187	0.9909	0.038*
C25	0.2254 (6)	0.8166 (6)	0.9917 (5)	0.0285 (14)
C26	0.1205 (6)	0.8471 (6)	0.9498 (5)	0.0308 (14)
H26	0.0431	0.8290	0.9713	0.037*
C27	0.1272 (6)	0.9054 (6)	0.8748 (5)	0.0269 (13)
C28	0.0182 (6)	0.9375 (6)	0.8317 (6)	0.0341 (15)
H28	−0.0588	0.9182	0.8532	0.041*
C29	0.0217 (6)	0.9958 (6)	0.7599 (5)	0.0320 (15)
H29	−0.0509	1.0163	0.7302	0.038*
C30	0.1372 (6)	1.0235 (6)	0.7324 (5)	0.0293 (14)
C31	0.2818 (6)	1.0986 (6)	0.6610 (5)	0.0262 (13)
C32	0.5543 (5)	0.9086 (6)	0.6865 (5)	0.0251 (13)
C33	0.6747 (6)	0.8905 (7)	0.7109 (5)	0.0346 (15)
H33	0.7220	0.9607	0.7620	0.041*
C34	0.7264 (6)	0.7704 (7)	0.6608 (6)	0.0371 (16)
H34	0.8091	0.7586	0.6780	0.045*
C35	0.6599 (7)	0.6687 (6)	0.5871 (6)	0.0372 (16)
H35	0.6958	0.5865	0.5530	0.045*
C36	0.5391 (7)	0.6866 (6)	0.5625 (6)	0.0372 (16)

H36	0.4927	0.6163	0.5108	0.045*
C37	0.4854 (6)	0.8059 (6)	0.6127 (5)	0.0306 (14)
H37	0.4022	0.8170	0.5965	0.037*
C38	0.3258 (6)	1.1671 (6)	0.5937 (5)	0.0328 (15)
H38A	0.3182	1.2614	0.6317	0.049*
H38B	0.2764	1.1376	0.5268	0.049*
H38C	0.4116	1.1475	0.5784	0.049*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0461 (4)	0.0292 (3)	0.0315 (4)	0.0040 (3)	0.0021 (3)	0.0168 (3)
Br2	0.0543 (5)	0.0316 (4)	0.0308 (4)	−0.0065 (3)	0.0025 (3)	0.0180 (3)
S1	0.0264 (8)	0.0206 (7)	0.0322 (9)	0.0028 (6)	0.0041 (6)	0.0099 (6)
S2	0.0259 (8)	0.0203 (7)	0.0341 (9)	−0.0029 (6)	0.0014 (6)	0.0096 (6)
O1	0.033 (2)	0.026 (2)	0.026 (2)	−0.0006 (17)	0.0070 (18)	0.0125 (18)
O2	0.032 (2)	0.027 (2)	0.031 (2)	0.0031 (18)	−0.0012 (18)	0.0158 (19)
C1	0.038 (3)	0.012 (3)	0.022 (3)	0.004 (2)	0.002 (3)	0.007 (2)
C2	0.028 (3)	0.017 (3)	0.023 (3)	0.000 (2)	0.006 (2)	0.006 (2)
C3	0.028 (3)	0.020 (3)	0.021 (3)	−0.004 (2)	0.001 (2)	0.002 (2)
C4	0.023 (3)	0.033 (3)	0.026 (3)	−0.002 (2)	0.002 (2)	0.014 (3)
C5	0.032 (3)	0.032 (3)	0.028 (3)	−0.006 (3)	0.005 (3)	0.012 (3)
C6	0.037 (4)	0.023 (3)	0.022 (3)	0.003 (3)	0.003 (3)	0.007 (3)
C7	0.034 (4)	0.028 (3)	0.023 (3)	0.003 (3)	0.000 (3)	0.007 (3)
C8	0.027 (3)	0.027 (3)	0.018 (3)	0.001 (2)	0.001 (2)	0.004 (2)
C9	0.027 (3)	0.032 (3)	0.021 (3)	0.000 (3)	−0.001 (2)	0.004 (3)
C10	0.025 (3)	0.036 (4)	0.031 (4)	−0.006 (3)	0.006 (3)	0.010 (3)
C11	0.037 (4)	0.021 (3)	0.016 (3)	−0.001 (2)	0.005 (3)	0.005 (2)
C12	0.031 (3)	0.021 (3)	0.029 (3)	0.001 (2)	0.003 (3)	0.008 (3)
C13	0.029 (3)	0.024 (3)	0.019 (3)	0.001 (2)	−0.005 (2)	0.010 (2)
C14	0.026 (3)	0.031 (3)	0.031 (4)	0.002 (3)	0.004 (3)	0.009 (3)
C15	0.032 (4)	0.037 (4)	0.046 (4)	−0.005 (3)	0.004 (3)	0.018 (3)
C16	0.046 (4)	0.028 (3)	0.032 (4)	−0.012 (3)	−0.007 (3)	0.008 (3)
C17	0.052 (4)	0.021 (3)	0.030 (4)	0.001 (3)	−0.008 (3)	0.008 (3)
C18	0.027 (3)	0.029 (3)	0.040 (4)	0.004 (3)	−0.002 (3)	0.014 (3)
C19	0.045 (4)	0.029 (3)	0.034 (4)	0.004 (3)	0.004 (3)	0.017 (3)
C20	0.027 (3)	0.016 (3)	0.022 (3)	−0.005 (2)	0.000 (2)	0.004 (2)
C21	0.025 (3)	0.019 (3)	0.030 (3)	−0.002 (2)	0.004 (3)	0.007 (3)
C22	0.031 (3)	0.019 (3)	0.020 (3)	−0.003 (2)	0.001 (2)	0.005 (2)
C23	0.032 (3)	0.026 (3)	0.036 (4)	−0.002 (3)	0.004 (3)	0.016 (3)
C24	0.037 (4)	0.026 (3)	0.032 (4)	0.003 (3)	0.000 (3)	0.012 (3)
C25	0.040 (4)	0.022 (3)	0.024 (3)	−0.005 (3)	0.001 (3)	0.010 (3)
C26	0.034 (4)	0.029 (3)	0.027 (3)	−0.004 (3)	0.007 (3)	0.007 (3)
C27	0.031 (3)	0.023 (3)	0.024 (3)	−0.005 (2)	0.002 (3)	0.006 (3)
C28	0.025 (3)	0.033 (3)	0.041 (4)	−0.002 (3)	0.005 (3)	0.011 (3)
C29	0.022 (3)	0.030 (3)	0.040 (4)	0.003 (3)	0.000 (3)	0.010 (3)
C30	0.030 (3)	0.028 (3)	0.032 (4)	0.004 (3)	0.004 (3)	0.013 (3)
C31	0.035 (3)	0.022 (3)	0.024 (3)	0.001 (2)	0.002 (3)	0.012 (3)

C32	0.025 (3)	0.023 (3)	0.033 (3)	0.002 (2)	0.010 (3)	0.017 (3)
C33	0.037 (4)	0.036 (4)	0.032 (4)	0.002 (3)	0.000 (3)	0.014 (3)
C34	0.034 (4)	0.048 (4)	0.035 (4)	0.013 (3)	0.007 (3)	0.023 (3)
C35	0.054 (4)	0.028 (3)	0.035 (4)	0.011 (3)	0.015 (3)	0.017 (3)
C36	0.048 (4)	0.027 (3)	0.036 (4)	−0.005 (3)	0.009 (3)	0.010 (3)
C37	0.032 (3)	0.030 (3)	0.033 (4)	−0.005 (3)	0.005 (3)	0.015 (3)
C38	0.048 (4)	0.022 (3)	0.034 (4)	−0.001 (3)	0.002 (3)	0.017 (3)

Geometric parameters (Å, °)

Br1—C6	1.904 (6)	C17—H17	0.9500
Br2—C25	1.903 (6)	C18—H18	0.9500
S1—C1	1.743 (6)	C19—H19A	0.9800
S1—C13	1.786 (6)	C19—H19B	0.9800
S2—C20	1.758 (6)	C19—H19C	0.9800
S2—C32	1.782 (6)	C20—C31	1.353 (8)
O1—C11	1.373 (7)	C20—C21	1.439 (8)
O1—C12	1.374 (7)	C21—C30	1.391 (9)
O2—C31	1.376 (8)	C21—C22	1.416 (8)
O2—C30	1.378 (7)	C22—C23	1.412 (9)
C1—C12	1.362 (8)	C22—C27	1.434 (8)
C1—C2	1.447 (8)	C23—C24	1.368 (9)
C2—C11	1.389 (8)	C23—H23	0.9500
C2—C3	1.422 (8)	C24—C25	1.409 (9)
C3—C4	1.420 (8)	C24—H24	0.9500
C3—C8	1.421 (8)	C25—C26	1.371 (9)
C4—C5	1.367 (9)	C26—C27	1.411 (9)
C4—H4	0.9500	C26—H26	0.9500
C5—C6	1.397 (9)	C27—C28	1.423 (9)
C5—H5	0.9500	C28—C29	1.37 (1)
C6—C7	1.356 (9)	C28—H28	0.9500
C7—C8	1.428 (9)	C29—C30	1.395 (9)
C7—H7	0.9500	C29—H29	0.9500
C8—C9	1.431 (9)	C31—C38	1.489 (8)
C9—C10	1.376 (9)	C32—C33	1.385 (9)
C9—H9	0.9500	C32—C37	1.385 (9)
C10—C11	1.385 (9)	C33—C34	1.385 (9)
C10—H10	0.9500	C33—H33	0.9500
C12—C19	1.475 (9)	C34—C35	1.37 (1)
C13—C18	1.375 (8)	C34—H34	0.9500
C13—C14	1.389 (9)	C35—C36	1.39 (1)
C14—C15	1.371 (9)	C35—H35	0.9500
C14—H14	0.9500	C36—C37	1.387 (9)
C15—C16	1.38 (1)	C36—H36	0.9500
C15—H15	0.9500	C37—H37	0.9500
C16—C17	1.37 (1)	C38—H38A	0.9800
C16—H16	0.9500	C38—H38B	0.9800
C17—C18	1.401 (9)	C38—H38C	0.9800
C1—S1—C13	105.9 (3)	H19A—C19—H19C	109.5

C20—S2—C32	103.8 (3)	H19B—C19—H19C	109.5
C11—O1—C12	106.9 (4)	C31—C20—C21	107.7 (5)
C31—O2—C30	106.2 (4)	C31—C20—S2	121.9 (5)
C12—C1—C2	107.1 (5)	C21—C20—S2	129.7 (5)
C12—C1—S1	122.1 (5)	C30—C21—C22	118.7 (5)
C2—C1—S1	130.3 (4)	C30—C21—C20	104.6 (5)
C11—C2—C3	118.2 (5)	C22—C21—C20	136.7 (6)
C11—C2—C1	105.0 (5)	C23—C22—C21	124.5 (6)
C3—C2—C1	136.8 (5)	C23—C22—C27	118.4 (5)
C4—C3—C8	118.7 (6)	C21—C22—C27	117.0 (5)
C4—C3—C2	123.7 (6)	C24—C23—C22	121.9 (6)
C8—C3—C2	117.6 (5)	C24—C23—H23	119.0
C5—C4—C3	121.1 (6)	C22—C23—H23	119.0
C5—C4—H4	119.4	C23—C24—C25	118.8 (6)
C3—C4—H4	119.4	C23—C24—H24	120.6
C4—C5—C6	119.4 (6)	C25—C24—H24	120.6
C4—C5—H5	120.3	C26—C25—C24	121.7 (6)
C6—C5—H5	120.3	C26—C25—Br2	119.6 (5)
C7—C6—C5	122.2 (6)	C24—C25—Br2	118.7 (5)
C7—C6—Br1	119.3 (5)	C25—C26—C27	120.1 (6)
C5—C6—Br1	118.5 (5)	C25—C26—H26	119.9
C6—C7—C8	119.8 (6)	C27—C26—H26	119.9
C6—C7—H7	120.1	C26—C27—C28	120.1 (6)
C8—C7—H7	120.1	C26—C27—C22	119.0 (6)
C3—C8—C7	118.8 (6)	C28—C27—C22	120.9 (6)
C3—C8—C9	120.8 (6)	C29—C28—C27	121.5 (6)
C7—C8—C9	120.4 (6)	C29—C28—H28	119.3
C10—C9—C8	121.1 (6)	C27—C28—H28	119.3
C10—C9—H9	119.4	C28—C29—C30	116.7 (6)
C8—C9—H9	119.4	C28—C29—H29	121.7
C9—C10—C11	116.7 (6)	C30—C29—H29	121.7
C9—C10—H10	121.6	O2—C30—C21	110.8 (5)
C11—C10—H10	121.6	O2—C30—C29	124.1 (6)
O1—C11—C10	123.9 (5)	C21—C30—C29	125.1 (6)
O1—C11—C2	110.5 (5)	C20—C31—O2	110.7 (5)
C10—C11—C2	125.5 (6)	C20—C31—C38	133.3 (6)
C1—C12—O1	110.4 (5)	O2—C31—C38	116.0 (5)
C1—C12—C19	133.8 (6)	C33—C32—C37	119.8 (6)
O1—C12—C19	115.7 (5)	C33—C32—S2	116.4 (5)
C18—C13—C14	120.8 (6)	C37—C32—S2	123.7 (5)
C18—C13—S1	123.9 (5)	C34—C33—C32	120.1 (6)
C14—C13—S1	115.4 (4)	C34—C33—H33	120.0
C15—C14—C13	119.4 (6)	C32—C33—H33	120.0
C15—C14—H14	120.3	C35—C34—C33	120.7 (6)
C13—C14—H14	120.3	C35—C34—H34	119.7
C14—C15—C16	121.1 (6)	C33—C34—H34	119.7
C14—C15—H15	119.4	C34—C35—C36	119.3 (6)
C16—C15—H15	119.4	C34—C35—H35	120.3
C17—C16—C15	119.0 (6)	C36—C35—H35	120.3

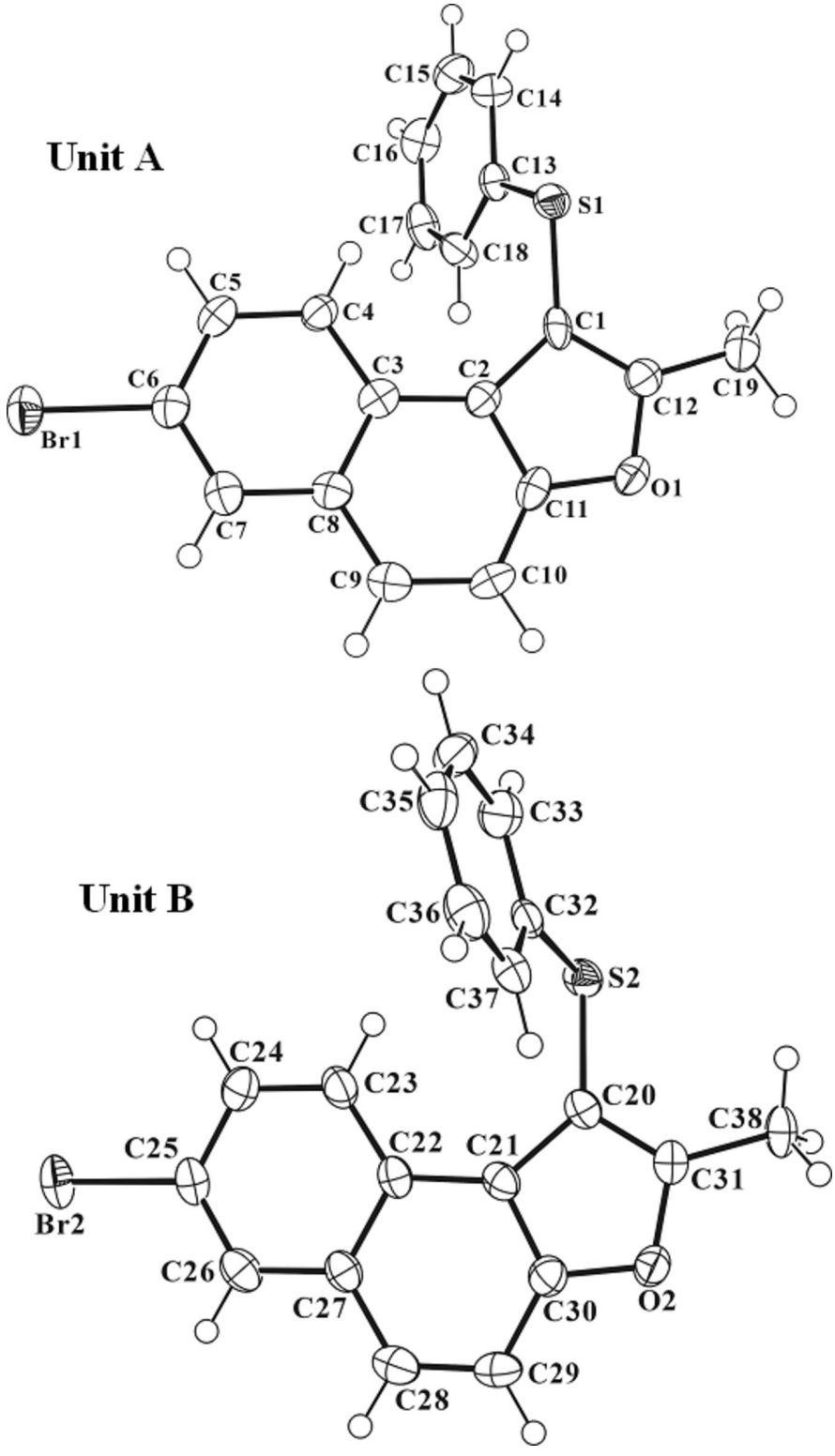
C17—C16—H16	120.5	C37—C36—C35	120.8 (6)
C15—C16—H16	120.5	C37—C36—H36	119.6
C16—C17—C18	121.4 (6)	C35—C36—H36	119.6
C16—C17—H17	119.3	C32—C37—C36	119.3 (6)
C18—C17—H17	119.3	C32—C37—H37	120.4
C13—C18—C17	118.3 (6)	C36—C37—H37	120.4
C13—C18—H18	120.8	C31—C38—H38A	109.5
C17—C18—H18	120.8	C31—C38—H38B	109.5
C12—C19—H19A	109.5	H38A—C38—H38B	109.5
C12—C19—H19B	109.5	C31—C38—H38C	109.5
H19A—C19—H19B	109.5	H38A—C38—H38C	109.5
C12—C19—H19C	109.5	H38B—C38—H38C	109.5
C13—S1—C1—C12	109.2 (5)	C32—S2—C20—C31	−111.8 (5)
C13—S1—C1—C2	−80.1 (6)	C32—S2—C20—C21	79.3 (6)
C12—C1—C2—C11	2.4 (6)	C31—C20—C21—C30	0.2 (7)
S1—C1—C2—C11	−169.4 (5)	S2—C20—C21—C30	170.3 (5)
C12—C1—C2—C3	−179.0 (7)	C31—C20—C21—C22	179.5 (7)
S1—C1—C2—C3	9.2 (11)	S2—C20—C21—C22	−10.4 (11)
C11—C2—C3—C4	−177.5 (6)	C30—C21—C22—C23	179.1 (6)
C1—C2—C3—C4	4.0 (11)	C20—C21—C22—C23	−0.1 (11)
C11—C2—C3—C8	0.8 (8)	C30—C21—C22—C27	−3.2 (8)
C1—C2—C3—C8	−177.7 (6)	C20—C21—C22—C27	177.6 (6)
C8—C3—C4—C5	0.6 (9)	C21—C22—C23—C24	177.7 (6)
C2—C3—C4—C5	178.9 (6)	C27—C22—C23—C24	−0.1 (9)
C3—C4—C5—C6	0.5 (9)	C22—C23—C24—C25	−0.8 (9)
C4—C5—C6—C7	−1.4 (10)	C23—C24—C25—C26	0.9 (9)
C4—C5—C6—Br1	179.7 (5)	C23—C24—C25—Br2	−179.2 (5)
C5—C6—C7—C8	1.0 (9)	C24—C25—C26—C27	−0.1 (9)
Br1—C6—C7—C8	179.9 (4)	Br2—C25—C26—C27	180.0 (5)
C4—C3—C8—C7	−1.0 (8)	C25—C26—C27—C28	−179.7 (6)
C2—C3—C8—C7	−179.3 (5)	C25—C26—C27—C22	−0.8 (9)
C4—C3—C8—C9	179.2 (6)	C23—C22—C27—C26	0.9 (8)
C2—C3—C8—C9	0.8 (8)	C21—C22—C27—C26	−177.0 (5)
C6—C7—C8—C3	0.1 (9)	C23—C22—C27—C28	179.8 (6)
C6—C7—C8—C9	−180.0 (6)	C21—C22—C27—C28	1.9 (8)
C3—C8—C9—C10	−1.0 (9)	C26—C27—C28—C29	179.1 (6)
C7—C8—C9—C10	179.1 (6)	C22—C27—C28—C29	0.2 (9)
C8—C9—C10—C11	−0.4 (9)	C27—C28—C29—C30	−0.9 (10)
C12—O1—C11—C10	−178.2 (6)	C31—O2—C30—C21	0.1 (7)
C12—O1—C11—C2	−0.3 (6)	C31—O2—C30—C29	177.8 (6)
C9—C10—C11—O1	179.7 (5)	C22—C21—C30—O2	−179.6 (5)
C9—C10—C11—C2	2.2 (9)	C20—C21—C30—O2	−0.2 (7)
C3—C2—C11—O1	179.8 (5)	C22—C21—C30—C29	2.7 (9)
C1—C2—C11—O1	−1.3 (6)	C20—C21—C30—C29	−177.9 (6)
C3—C2—C11—C10	−2.4 (9)	C28—C29—C30—O2	−178.0 (6)
C1—C2—C11—C10	176.5 (6)	C28—C29—C30—C21	−0.6 (10)
C2—C1—C12—O1	−2.7 (6)	C21—C20—C31—O2	−0.2 (7)
S1—C1—C12—O1	169.9 (4)	S2—C20—C31—O2	−171.2 (4)
C2—C1—C12—C19	179.5 (7)	C21—C20—C31—C38	177.8 (6)

S1—C1—C12—C19	−7.9 (10)	S2—C20—C31—C38	6.7 (10)
C11—O1—C12—C1	1.9 (6)	C30—O2—C31—C20	0.1 (6)
C11—O1—C12—C19	−179.8 (5)	C30—O2—C31—C38	−178.3 (5)
C1—S1—C13—C18	5.5 (6)	C20—S2—C32—C33	−168.5 (5)
C1—S1—C13—C14	−173.8 (5)	C20—S2—C32—C37	12.8 (6)
C18—C13—C14—C15	−0.7 (10)	C37—C32—C33—C34	0.6 (10)
S1—C13—C14—C15	178.7 (5)	S2—C32—C33—C34	−178.1 (5)
C13—C14—C15—C16	−0.1 (10)	C32—C33—C34—C35	0.0 (10)
C14—C15—C16—C17	0.0 (11)	C33—C34—C35—C36	0.0 (10)
C15—C16—C17—C18	0.8 (10)	C34—C35—C36—C37	−0.6 (10)
C14—C13—C18—C17	1.4 (9)	C33—C32—C37—C36	−1.2 (9)
S1—C13—C18—C17	−177.9 (5)	S2—C32—C37—C36	177.4 (5)
C16—C17—C18—C13	−1.5 (10)	C35—C36—C37—C32	1.3 (10)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C19—H19C···Cg3	0.98	2.77	3.551 (6)	137
C38—H38A···Cg5	0.98	2.60	3.498 (6)	153

Fig. 1


Unit A
C15
C14
C16
C13
S1
C17
C18
C5
C4
C1
C6
C3
C2
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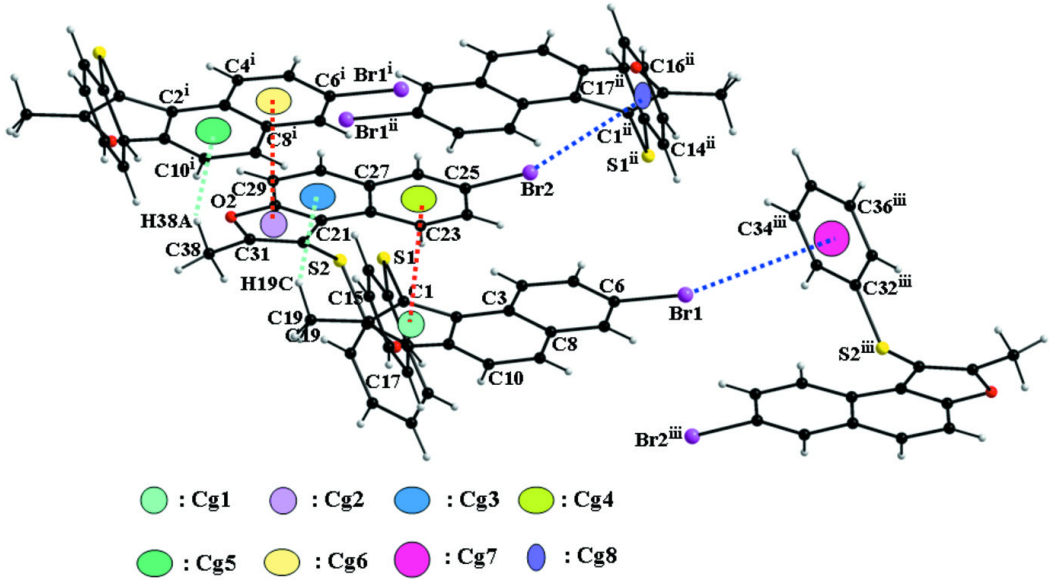
C19
Br1
O1
C11
C7
C8
C9
C10
Unit B
C34
C35
C33
C36
C32
S2
C37
C24
C23
C20
C38
C25
C22
C21
C31
Br2
C26
C27
C30
O2
C29
C28

Fig. 2


C4i
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Br1i
C2i
C16ii
C17ii
C8i
Br1ii
C1ii
C14ii
S1ii
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C27
C25
Br2
O2
H38A
C21
C23
C38
C31
S1
S2
H19C
C15
C1
C3
C6
Br1
C19
C18
C8
C17
C10
C34iii
C36iii
C32iii
S2iii
Br2iii
: Cg1
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: Cg3
: Cg4
: Cg5
: Cg6
: Cg7
: Cg8