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(2*E*)-1-(3-Bromothien-2-yl)-3-phenylprop-2-en-1-one

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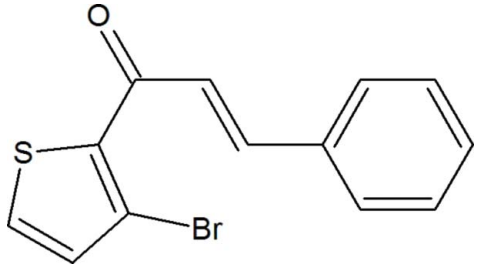
Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.011 Å; R factor = 0.069; wR factor = 0.178; data-to-parameter ratio = 19.3.

The title compound, $C_{13}H_9BrOS$, crystallizes with two independent molecules (*A* and *B*) in the asymmetric unit. The mean planes of the 3-bromothien-2-yl and 3-phenyl groups in *A* and *B* form dihedral angles of 4.9 (7) and 12.2 (4)°, respectively. The angles between the mean plane of the prop-2-en-1-one group and those of the 3-bromothien-2-yl and 3-phenyl groups are 2.8 (2) and 3.8 (2)°, respectively, in molecule *A*, and 5.1 (1) and 9.8 (9)° in molecule *B*. Essentially planar groups of molecule *A* pack zigzag to similar groups of molecule *B* along the *a* axis of the unit cell.

Related literature

For related structures, see: Baxter *et al.* (1990); Ng *et al.* (2006); Yathirajan, Sarojini, Narayana, Ashalatha & Bolte (2006); Yathirajan, Sarojini, Narayana, Bindya & Bolte (2006); Harrison *et al.* (2006); Butcher *et al.* (2007*a*,*b*,*c*). For related background, see: Fichou *et al.* (1988); Goto *et al.* (1991); Cho *et al.* (1996); Uchida *et al.* (1998); Tam *et al.* (1989); Indira *et al.* (2002); Opletalova & Sedivy (1999); Butcher, Yathirajan, Sarojini *et al.* (2006); Butcher *et al.* (2006*a*,*b*).



Experimental

Crystal data

$C_{13}H_9BrOS$
M_r = 293.17
Orthorhombic, $Pca2_1$
a = 17.321 (4) Å
b = 5.4295 (12) Å
c = 24.600 (5) Å
V = 2313.5 (9) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 3.71 mm^{-1}
T = 123 K
0.69 × 0.32 × 0.10 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.335, T_{max} = 1.000
(expected range = 0.236–0.703)
17031 measured reflections
5590 independent reflections
4041 reflections with $I > 2\sigma(I)$
R_{int} = 0.105

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.178
S = 0.99
5590 reflections
289 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.41 e Å^{-3}
$\Delta\rho_{min}$ = −1.49 e Å^{-3}
Absolute structure: Flack (1983), with 2580 Friedel pairs
Flack parameter: 0.014 (15)

Data collection: *APEX2* (Bruker, 2006); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL* (Bruker, 2000).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2454).

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supplementary materials

Acta Cryst. (2007). E**63**, o3705-o3706 [**doi:10.1107/S1600536807037841**]

(2*E*)-1-(3-Bromothien-2-yl)-3-phenylprop-2-en-1-one

R. J. Butcher, J. P. Jasinski, H. S. Yathirajan, B. V. Ashalatha and B. Narayana

Comment

Chalcones and their heterocyclic derivatives show numerous biological effects. Among several organic compounds reported for non-linear optical (NLO) property, chalcone derivatives are noticeable materials for their excellent blue light transmittance and good crystallizability. Chalcones provide a necessary configuration to show NLO property with two planar rings connected through a conjugated double bond. The NLO effect in organic molecules originates from a strong intermolecular donor-acceptor interaction, a delocalized π-electron system, and the ability to crystallize in a non-centrosymmetric structure. Secondly, the backbone is usually twisted, and this twist is inherently chiral and often results in these compounds crystallizing in non-centrosymmetric space groups. Substitution on either of the phenyl rings greatly influences non-centrosymmetric crystal packing. It is speculated that, in order to improve the activity, more bulky substituents should be introduced to increase the spontaneous polarization of a non-centrosymmetric crystal structure The molecular hyperpolarizability, β, is strongly influenced not only by the electronic effect, but also by the steric effect of the subsistent. Prompted by this, and in continuation of our quest to synthesize new materials which can find use in the photonics industries, we have synthesized a new chalcone and the present paper reports the crystal structure of a newly synthesized chalcone, (I), $C_{13}H_9BrOS$.

The mean planes of the 3-Bromothien-2-yl and 3-phenyl groups in molecules A and B form dihedral angles of 4.9 (7)° and 12.2 (4)°, respectively, with each other (Fig. 1). The angles between the mean plane of the prop-2-en-1-one group and those of the 3-Bromothien-2-yl and 3-phenyl groups are 2.8 (2)° and 3.8 (2)° in molecule A, and 5.1 (1)° and 9.8 (9)° in molecule B.

The packing diagram displays a zigzag array of mean planes of adjacent planar arranged groups of molecules A located next to mean planes of molecules B located diagonal along the *a* axis of the unit cell (Fig. 2). The closest centroid-centroid distance of 4.63 (2) Å occurs between the nearby mean planes of the inverted 3-Bromothien-2-yl and 3-phenyl groups for molecule A.

Experimental

3-bromo-2-acetylthiophene (10 g, 0.048 mol) in 50 ml me thanol is mixed with benzaldehyde (5.0 g, 0.048 mol) and the mixture was treated with an 10 ml of 30% potassium hydroxide solution at 278 K (Fig. 3). The reaction mixture was then brought to room temperature and stirred for 3 h. The solid precipated was filtered and washed with water, dried and recrytallized from toluene (m.p.: 339 K).

Refinement

The high value of R_{int} is probably due to poor crystal quality. The H atoms were included in the riding model approximation with C—H = 0.95 Å, and with U_{iso}(H) = 1.18–1.21U_{eq}(C). The maximum residual electron density peaks of 2.40 and −1.49 e Å^3, were located at 0.90 and 0.76 Å from the Br1A and Br1B atoms, respectively.

Figures

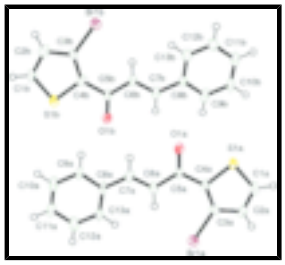


Fig. 1. Molecular structure of $C_{13}H_9BrOS$, (I), showing atom labeling and 50% probability displacement ellipsoids for independent molecules A and B in the asymmetric unit.

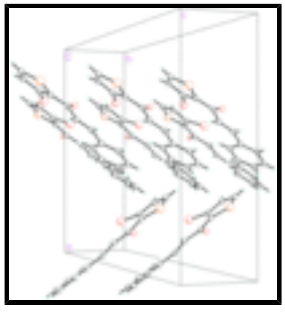


Fig. 2. Packing diagram of $C_{13}H_9BrOS$ viewed down the *b* axis.

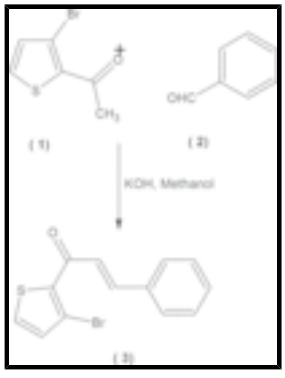


Fig. 3. Synthesis scheme of $C_{13}H_9BrOS$.

(2E)-1-(3-Bromothien-2-yl)-3-phenylprop-2-en-1-one

Crystal data

$C_{13}H_9BrOS$	$D_x = 1.683$ Mg m^{-3}
$M_r = 293.17$	Mo *K*α radiation λ = 0.71073 Å
Orthorhombic, *Pca*2$_1$	Cell parameters from 5433 reflections
a = 17.321 (4) Å	θ = 2.4–28.3°
b = 5.4295 (12) Å	μ = 3.71 mm^{-1}
c = 24.600 (5) Å	*T* = 123 K
V = 2313.5 (9) Å^3	Rectangular, colourless
Z = 8	0.69 × 0.32 × 0.10 mm
F_{000} = 1168	

Data collection

Bruker APEXII CCD area-detector diffractometer	5590 independent reflections
Radiation source: fine-focus sealed tube	4041 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.105$
$T = 123$ K	$\theta_{max} = 28.7^{o}$
φ and ω scans	$\theta_{min} = 2.4^{o}$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -23 \rightarrow 23$
$T_{min} = 0.335$, $T_{max} = 1.000$	$k = -5 \rightarrow 7$
17031 measured reflections	$l = -31 \rightarrow 33$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.069$	$w = 1/[\sigma^2(F_o^2) + (0.114P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.178$	$(\Delta/\sigma)_{max} = 0.001$
$S = 0.99$	$\Delta\rho_{max} = 2.41$ e Å^{-3}
5590 reflections	$\Delta\rho_{min} = -1.49$ e Å^{-3}
289 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), 2580 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.014 (15)
Secondary atom site location: difference Fourier map	

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}
Br1A	0.19487 (4)	−0.04060 (15)	0.04400 (3)	0.0344 (2)
Br1B	−0.10871 (5)	0.54938 (16)	0.45589 (3)	0.0362 (2)
S1A	0.25796 (9)	−0.2937 (3)	0.20837 (8)	0.0247 (4)

S1B	−0.15628 (9)	0.7896 (3)	0.28805 (8)	0.0242 (4)
O1A	0.1645 (3)	0.1132 (10)	0.2363 (2)	0.0248 (10)
O1B	−0.0611 (3)	0.3863 (11)	0.2652 (2)	0.0309 (12)
C1A	0.2977 (4)	−0.4717 (15)	0.1588 (4)	0.0274 (17)
H1AA	0.3305	−0.6085	0.1656	0.033*
C2A	0.2771 (4)	−0.3951 (16)	0.1081 (3)	0.0291 (17)
H2AA	0.2935	−0.4729	0.0755	0.035*
C3A	0.2279 (4)	−0.1846 (13)	0.1098 (3)	0.0218 (14)
C4A	0.2109 (4)	−0.1080 (15)	0.1615 (3)	0.0224 (15)
C5A	0.1631 (3)	0.0939 (14)	0.1870 (3)	0.0220 (15)
C6A	0.1159 (3)	0.2476 (14)	0.1517 (3)	0.0233 (15)
H6AA	0.1161	0.2209	0.1135	0.028*
C7A	0.0719 (4)	0.4273 (14)	0.1731 (3)	0.0258 (16)
H7AA	0.0741	0.4479	0.2114	0.031*
C8A	0.0203 (4)	0.5969 (14)	0.1426 (3)	0.0234 (15)
C9A	−0.0133 (3)	0.7948 (14)	0.1707 (4)	0.0282 (16)
H9AA	−0.0033	0.8184	0.2083	0.034*
C10A	−0.0618 (4)	0.9568 (14)	0.1427 (4)	0.0323 (19)
H10A	−0.0856	1.0885	0.1617	0.039*
C11A	−0.0754 (4)	0.9286 (14)	0.0882 (4)	0.0329 (19)
H11A	−0.1064	1.0446	0.0693	0.040*
C12A	−0.0432 (4)	0.7272 (16)	0.0604 (3)	0.0350 (19)
H12A	−0.0541	0.7031	0.0229	0.042*
C13A	0.0046 (4)	0.5632 (16)	0.0877 (3)	0.0321 (18)
H13A	0.0267	0.4278	0.0688	0.039*
C1B	−0.1999 (4)	0.9667 (14)	0.3363 (4)	0.0276 (16)
H1BA	−0.2330	1.1005	0.3276	0.033*
C2B	−0.1839 (4)	0.9028 (15)	0.3871 (3)	0.0253 (16)
H2BA	−0.2026	0.9852	0.4185	0.030*
C3B	−0.1345 (4)	0.6920 (14)	0.3877 (3)	0.0243 (14)
C4B	−0.1132 (3)	0.6062 (15)	0.3372 (3)	0.0220 (15)
C5B	−0.0641 (4)	0.4081 (12)	0.3151 (3)	0.0206 (14)
C6B	−0.0212 (4)	0.2400 (15)	0.3516 (3)	0.0272 (16)
H6BA	−0.0264	0.2568	0.3899	0.033*
C7B	0.0246 (4)	0.0655 (14)	0.3314 (3)	0.0250 (15)
H7BA	0.0260	0.0508	0.2929	0.030*
C8B	0.0732 (3)	−0.1073 (13)	0.3625 (3)	0.0252 (16)
C9B	0.1140 (4)	−0.2874 (13)	0.3332 (3)	0.0254 (15)
H9BA	0.1109	−0.2924	0.2946	0.030*
C10B	0.1595 (4)	−0.4607 (15)	0.3615 (4)	0.0330 (18)
H10B	0.1873	−0.5822	0.3417	0.040*
C11B	0.1642 (4)	−0.4563 (15)	0.4168 (4)	0.0354 (19)
H11B	0.1947	−0.5741	0.4356	0.042*
C12B	0.1238 (5)	−0.2768 (18)	0.4451 (4)	0.046 (2)
H12B	0.1277	−0.2700	0.4836	0.055*
C13B	0.0778 (5)	−0.1073 (16)	0.4182 (4)	0.0320 (17)
H13B	0.0492	0.0102	0.4385	0.038*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1A	0.0368 (4)	0.0379 (5)	0.0284 (4)	0.0097 (3)	−0.0013 (3)	0.0006 (4)
Br1B	0.0410 (4)	0.0391 (5)	0.0286 (4)	0.0139 (3)	0.0015 (3)	0.0031 (5)
S1A	0.0172 (7)	0.0230 (9)	0.0340 (9)	0.0013 (6)	−0.0024 (6)	0.0024 (8)
S1B	0.0190 (7)	0.0232 (9)	0.0303 (9)	0.0022 (6)	−0.0020 (6)	−0.0003 (7)
O1A	0.020 (2)	0.022 (3)	0.032 (3)	0.003 (2)	0.003 (2)	0.001 (2)
O1B	0.031 (3)	0.027 (3)	0.034 (3)	0.011 (2)	0.004 (2)	0.001 (2)
C1A	0.009 (3)	0.028 (4)	0.045 (5)	0.005 (3)	−0.002 (3)	−0.002 (3)
C2A	0.017 (3)	0.033 (5)	0.037 (4)	−0.005 (3)	0.000 (3)	−0.004 (3)
C3A	0.021 (3)	0.017 (4)	0.027 (4)	0.000 (2)	−0.003 (3)	0.006 (3)
C4A	0.018 (3)	0.021 (4)	0.029 (4)	−0.008 (3)	0.002 (3)	−0.008 (3)
C5A	0.007 (2)	0.026 (4)	0.034 (4)	0.001 (2)	0.001 (2)	0.002 (3)
C6A	0.017 (3)	0.021 (4)	0.031 (4)	0.003 (3)	0.000 (3)	−0.001 (3)
C7A	0.016 (3)	0.022 (4)	0.040 (4)	0.001 (2)	−0.002 (3)	0.001 (3)
C8A	0.013 (3)	0.022 (4)	0.035 (4)	0.000 (2)	0.002 (3)	0.003 (3)
C9A	0.012 (3)	0.021 (4)	0.051 (5)	−0.004 (3)	0.002 (3)	−0.001 (3)
C10A	0.014 (3)	0.020 (4)	0.063 (6)	0.003 (3)	0.007 (3)	0.011 (4)
C11A	0.019 (3)	0.020 (4)	0.060 (6)	0.001 (3)	0.000 (3)	0.014 (4)
C12A	0.029 (3)	0.038 (5)	0.038 (5)	0.005 (3)	0.000 (3)	0.011 (3)
C13A	0.027 (3)	0.030 (5)	0.040 (5)	0.004 (3)	0.003 (3)	0.004 (4)
C1B	0.018 (3)	0.020 (4)	0.045 (5)	0.000 (3)	−0.002 (3)	−0.001 (3)
C2B	0.015 (3)	0.025 (4)	0.035 (4)	−0.005 (3)	0.007 (3)	−0.006 (3)
C3B	0.023 (3)	0.021 (4)	0.028 (4)	−0.007 (3)	−0.003 (3)	0.003 (3)
C4B	0.008 (2)	0.022 (4)	0.036 (4)	0.000 (2)	0.002 (2)	0.006 (3)
C5B	0.021 (3)	0.007 (3)	0.034 (4)	−0.002 (2)	0.000 (3)	−0.003 (3)
C6B	0.020 (3)	0.030 (4)	0.032 (4)	0.005 (3)	−0.005 (3)	0.000 (3)
C7B	0.014 (3)	0.025 (4)	0.036 (4)	0.001 (3)	−0.002 (3)	−0.001 (3)
C8B	0.012 (3)	0.011 (3)	0.053 (5)	0.003 (2)	−0.003 (3)	−0.004 (3)
C9B	0.018 (3)	0.012 (3)	0.046 (4)	0.000 (2)	0.004 (3)	−0.001 (3)
C10B	0.014 (3)	0.025 (4)	0.060 (6)	0.003 (3)	0.001 (3)	0.001 (4)
C11B	0.020 (3)	0.030 (5)	0.056 (6)	0.009 (3)	−0.003 (3)	0.004 (4)
C12B	0.050 (5)	0.038 (5)	0.050 (6)	0.019 (4)	−0.009 (4)	0.006 (4)
C13B	0.033 (4)	0.023 (4)	0.039 (4)	0.015 (3)	−0.009 (3)	−0.008 (3)

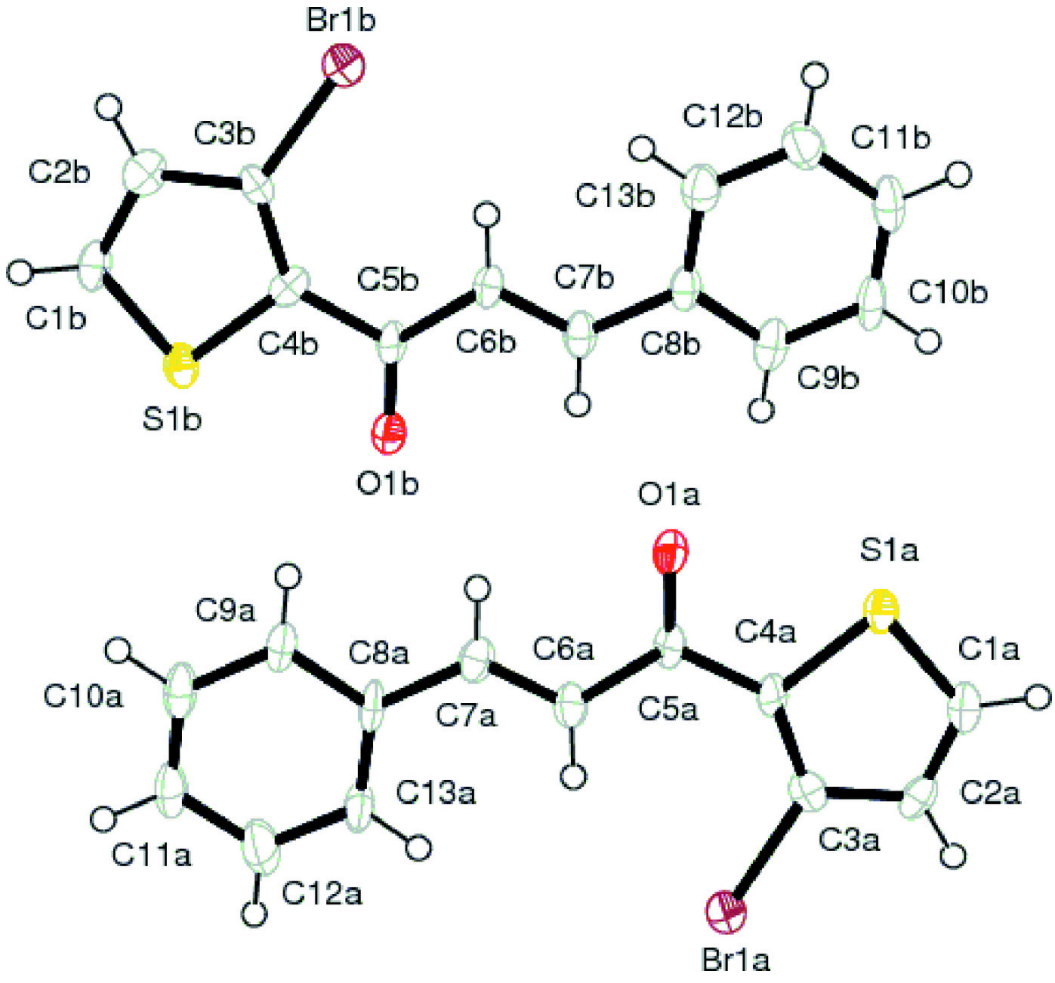
Geometric parameters (Å, °)

Br1A—C3A	1.886 (7)	C11A—H11A	0.9500
Br1B—C3B	1.900 (7)	C12A—C13A	1.389 (11)
S1A—C1A	1.702 (8)	C12A—H12A	0.9500
S1A—C4A	1.736 (8)	C13A—H13A	0.9500
S1B—C1B	1.705 (8)	C1B—C2B	1.324 (12)
S1B—C4B	1.735 (8)	C1B—H1BA	0.9500
O1A—C5A	1.216 (9)	C2B—C3B	1.429 (11)
O1B—C5B	1.235 (9)	C2B—H2BA	0.9500
C1A—C2A	1.361 (12)	C3B—C4B	1.378 (11)
C1A—H1AA	0.9500	C4B—C5B	1.475 (10)

C2A—C3A	1.426 (10)	C5B—C6B	1.480 (10)
C2A—H2AA	0.9500	C6B—C7B	1.332 (10)
C3A—C4A	1.371 (10)	C6B—H6BA	0.9500
C4A—C5A	1.510 (10)	C7B—C8B	1.476 (10)
C5A—C6A	1.457 (10)	C7B—H7BA	0.9500
C6A—C7A	1.345 (10)	C8B—C13B	1.371 (12)
C6A—H6AA	0.9500	C8B—C9B	1.406 (10)
C7A—C8A	1.487 (10)	C9B—C10B	1.412 (11)
C7A—H7AA	0.9500	C9B—H9BA	0.9500
C8A—C13A	1.390 (11)	C10B—C11B	1.363 (13)
C8A—C9A	1.403 (10)	C10B—H10B	0.9500
C9A—C10A	1.397 (11)	C11B—C12B	1.388 (12)
C9A—H9AA	0.9500	C11B—H11B	0.9500
C10A—C11A	1.370 (13)	C12B—C13B	1.386 (11)
C10A—H10A	0.9500	C12B—H12B	0.9500
C11A—C12A	1.405 (12)	C13B—H13B	0.9500
C1A—S1A—C4A	92.5 (4)	C8A—C13A—H13A	119.9
C1B—S1B—C4B	91.7 (4)	C2B—C1B—S1B	114.6 (6)
C2A—C1A—S1A	112.1 (6)	C2B—C1B—H1BA	122.7
C2A—C1A—H1AA	123.9	S1B—C1B—H1BA	122.7
S1A—C1A—H1AA	123.9	C1B—C2B—C3B	110.2 (7)
C1A—C2A—C3A	112.0 (7)	C1B—C2B—H2BA	124.9
C1A—C2A—H2AA	124.0	C3B—C2B—H2BA	124.9
C3A—C2A—H2AA	124.0	C4B—C3B—C2B	114.9 (7)
C4A—C3A—C2A	113.5 (6)	C4B—C3B—Br1B	126.5 (6)
C4A—C3A—Br1A	127.2 (6)	C2B—C3B—Br1B	118.5 (6)
C2A—C3A—Br1A	119.3 (5)	C3B—C4B—C5B	137.1 (7)
C3A—C4A—C5A	136.4 (7)	C3B—C4B—S1B	108.6 (6)
C3A—C4A—S1A	109.8 (6)	C5B—C4B—S1B	114.2 (6)
C5A—C4A—S1A	113.7 (5)	O1B—C5B—C4B	117.4 (6)
O1A—C5A—C6A	123.8 (6)	O1B—C5B—C6B	121.5 (6)
O1A—C5A—C4A	117.8 (6)	C4B—C5B—C6B	121.1 (6)
C6A—C5A—C4A	118.3 (7)	C7B—C6B—C5B	120.7 (7)
C7A—C6A—C5A	120.0 (7)	C7B—C6B—H6BA	119.6
C7A—C6A—H6AA	120.0	C5B—C6B—H6BA	119.6
C5A—C6A—H6AA	120.0	C6B—C7B—C8B	126.8 (8)
C6A—C7A—C8A	126.4 (7)	C6B—C7B—H7BA	116.6
C6A—C7A—H7AA	116.8	C8B—C7B—H7BA	116.6
C8A—C7A—H7AA	116.8	C13B—C8B—C9B	118.9 (7)
C13A—C8A—C9A	119.9 (7)	C13B—C8B—C7B	123.5 (7)
C13A—C8A—C7A	121.7 (7)	C9B—C8B—C7B	117.5 (7)
C9A—C8A—C7A	118.4 (7)	C8B—C9B—C10B	119.4 (8)
C10A—C9A—C8A	119.2 (8)	C8B—C9B—H9BA	120.3
C10A—C9A—H9AA	120.4	C10B—C9B—H9BA	120.3
C8A—C9A—H9AA	120.4	C11B—C10B—C9B	120.9 (7)
C11A—C10A—C9A	121.1 (8)	C11B—C10B—H10B	119.5
C11A—C10A—H10A	119.5	C9B—C10B—H10B	119.5
C9A—C10A—H10A	119.5	C10B—C11B—C12B	118.9 (8)
C10A—C11A—C12A	119.6 (7)	C10B—C11B—H11B	120.5

C10A—C11A—H11A	120.2	C12B—C11B—H11B	120.5
C12A—C11A—H11A	120.2	C13B—C12B—C11B	121.1 (9)
C13A—C12A—C11A	120.0 (8)	C13B—C12B—H12B	119.5
C13A—C12A—H12A	120.0	C11B—C12B—H12B	119.5
C11A—C12A—H12A	120.0	C8B—C13B—C12B	120.7 (8)
C12A—C13A—C8A	120.1 (8)	C8B—C13B—H13B	119.6
C12A—C13A—H13A	119.9	C12B—C13B—H13B	119.6
C4A—S1A—C1A—C2A	0.3 (6)	C4B—S1B—C1B—C2B	1.1 (6)
S1A—C1A—C2A—C3A	0.4 (8)	S1B—C1B—C2B—C3B	−1.6 (8)
C1A—C2A—C3A—C4A	−1.2 (9)	C1B—C2B—C3B—C4B	1.4 (9)
C1A—C2A—C3A—Br1A	178.0 (5)	C1B—C2B—C3B—Br1B	−175.8 (5)
C2A—C3A—C4A—C5A	−179.2 (7)	C2B—C3B—C4B—C5B	178.3 (7)
Br1A—C3A—C4A—C5A	1.6 (12)	Br1B—C3B—C4B—C5B	−4.8 (12)
C2A—C3A—C4A—S1A	1.4 (7)	C2B—C3B—C4B—S1B	−0.6 (7)
Br1A—C3A—C4A—S1A	−177.7 (4)	Br1B—C3B—C4B—S1B	176.3 (4)
C1A—S1A—C4A—C3A	−1.0 (5)	C1B—S1B—C4B—C3B	−0.2 (5)
C1A—S1A—C4A—C5A	179.5 (5)	C1B—S1B—C4B—C5B	−179.4 (5)
C3A—C4A—C5A—O1A	−176.5 (7)	C3B—C4B—C5B—O1B	178.2 (8)
S1A—C4A—C5A—O1A	2.8 (8)	S1B—C4B—C5B—O1B	−2.9 (8)
C3A—C4A—C5A—C6A	5.9 (12)	C3B—C4B—C5B—C6B	−0.8 (12)
S1A—C4A—C5A—C6A	−174.8 (5)	S1B—C4B—C5B—C6B	178.1 (5)
O1A—C5A—C6A—C7A	1.8 (11)	O1B—C5B—C6B—C7B	2.7 (11)
C4A—C5A—C6A—C7A	179.2 (6)	C4B—C5B—C6B—C7B	−178.3 (7)
C5A—C6A—C7A—C8A	−179.3 (6)	C5B—C6B—C7B—C8B	177.1 (7)
C6A—C7A—C8A—C13A	8.7 (11)	C6B—C7B—C8B—C13B	−0.6 (12)
C6A—C7A—C8A—C9A	−171.5 (7)	C6B—C7B—C8B—C9B	176.4 (7)
C13A—C8A—C9A—C10A	−0.5 (10)	C13B—C8B—C9B—C10B	−1.0 (10)
C7A—C8A—C9A—C10A	179.7 (6)	C7B—C8B—C9B—C10B	−178.2 (6)
C8A—C9A—C10A—C11A	−1.6 (10)	C8B—C9B—C10B—C11B	0.2 (11)
C9A—C10A—C11A—C12A	3.0 (11)	C9B—C10B—C11B—C12B	−0.4 (12)
C10A—C11A—C12A—C13A	−2.5 (11)	C10B—C11B—C12B—C13B	1.4 (13)
C11A—C12A—C13A—C8A	0.4 (12)	C9B—C8B—C13B—C12B	2.1 (12)
C9A—C8A—C13A—C12A	1.0 (11)	C7B—C8B—C13B—C12B	179.1 (8)
C7A—C8A—C13A—C12A	−179.2 (7)	C11B—C12B—C13B—C8B	−2.3 (14)

Fig. 1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Br1a

Fig. 2

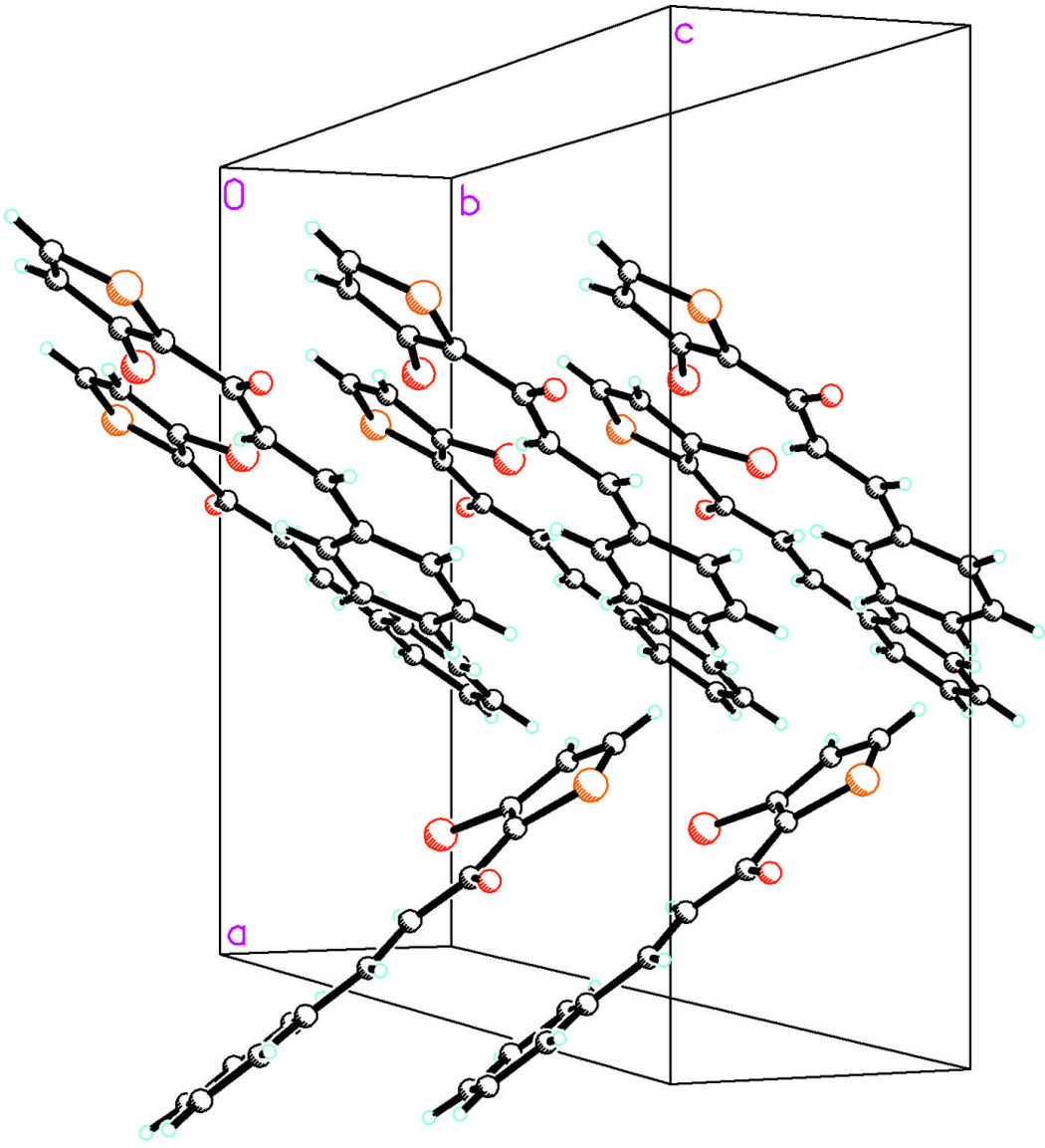

Fig. 3