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1-(4-Bromophenyl)-3-(3-methyl-2-thienyl)prop-2-en-1-one

Hoong-Kun Fun,[a]* Suchada Chantrapromma,[b]‡ P. S. Patil[c] and S. M. Dharmaprakash[c]

[a]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, [b]Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat-Yai, Songkhla 90112, Thailand, and [c]Department of Studies in Physics, Mangalore University, Mangalagangotri, Mangalore 574 199, India
Correspondence e-mail: hkfun@usm.my

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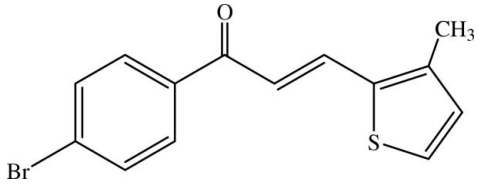
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.038; wR factor = 0.108; data-to-parameter ratio = 23.3.

The title compound, $C_{14}H_{11}BrOS$, crystallizes with four independent molecules (*A*, *B*, *C* and *D*) in the asymmetric unit which differ in the orientations of the thiophene and benzene rings with respect to the enone unit. The dihedral angles between the benzene and thiophene rings are 6.03 (14), 21.79 (14), 15.04 (14) and 4.92 (14)°, respectively, in molecules *A*, *B*, *C* and *D*. Intramolecular C—H···O and C—H···S interactions generate *S*(5) ring motifs. In the crystal structure, weak C—H···O intermolecular hydrogen bonds link the molecules into layers parallel to the [011] plane. In addition, short intermolecular Br···O contacts [2.997 (2)–3.110 (2) Å] are observed.

Related literature

For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For bond-length data see: Allen *et al.* (1987). For related structures, see: Patil, Dharmaprakash *et al.* (2006); Patil, Ng *et al.* (2007); Patil, Rosli *et al.* (2007); Patil, Teh *et al.* (2006); Patil, Teh *et al.* (2007); Shettigar *et al.* (2006); Patil, Chantrapromma *et al.* (2007).



Experimental

Crystal data

$C_{14}H_{11}BrOS$
M_r = 307.20
Triclinic, $P\overline{1}$
a = 7.4329 (3) Å
b = 17.3541 (7) Å
c = 19.2551 (8) Å
α = 90.736 (2)°
β = 90.731 (2)°
γ = 93.942 (2)°
V = 2477.43 (17) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 3.47 mm^{-1}
T = 100.0 (1) K
0.56 × 0.54 × 0.34 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.165, T_{max} = 0.307
42459 measured reflections
14381 independent reflections
10457 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.108
S = 1.06
14381 reflections
617 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.91 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C1A—H1A···O1C^{i}	0.93	2.55	3.478 (4)	175
C1B—H1B···O1D^{ii}	0.93	2.47	3.397 (4)	177
C1D—H1D···O1B^{iii}	0.93	2.54	3.440 (4)	164

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $-x+1, -y+1, -z$; (iii) $-x, -y+2, -z$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2377).

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‡ Additional correspondence author, email: suchada.c@psu.ac.th

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supplementary materials

Acta Cryst. (2007). E**63**, o2724-o2725 [**doi:10.1107/S1600536807020089**]

1-(4-Bromophenyl)-3-(3-methyl-2-thienyl)prop-2-en-1-one

H.-K. Fun, S. Chantrapromma, P. S. Patil and S. M. Dharmaprakash

Comment

Chalcone derivatives play an important role in non-linear optics (Patil, Dharmaprakash *et al.*, 2006; Patil, Chantrapromma *et al.*, 2007; Patil, Teh *et al.*, 2006, 2007). We have synthesized a series of chalcone derivatives to study their non-linear optical properties (Patil, Teh *et al.*, 2006; 2007; Patil, Dharmaprakash *et al.*, 2006; Shettigar *et al.*, 2006; Patil, Ng *et al.*, 2007; Patil, Rosli *et al.*, 2007; Patil, Chantrapromma *et al.*, 2007). Now we report here the crystal and molecular structure of the title compound, (I). Compound (I) crystallizes in a centrosymmetric space group and hence this precludes the presence of second-order non-linear optical properties.

Compound (I) crystallizes with four independent molecules (*A*, *B*, *C* and *D*) per asymmetric unit (Fig. 1). The dimensions of all four molecules are very similar, except for slightly different orientations of the thiophene and benzene rings with respect to the enone unit [C5–C7/O1]. The dihedral angles between the benzene and thiophene rings in molecules *A*, *B*, *C* and *D* are 6.03 (14)°, 21.79 (14)°, 15.04 (14)° and 4.92 (14)°, respectively. The enone unit in each molecule is slighly distorted from planarity, as indicated by the C5–C6–C7–O1 torsion angles of 2.8 (5)°, -3.9 (4)°, -4.7 (4) and 2.3 (4)°, respectively, in molecules *A*, *B*, *C* and *D*. The bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987) and comparable to those in related structures (Patil, Teh *et al.*, 2006; Patil, Dharmaprakash *et al.*, 2006; Shettigar *et al.*, 2006; Patil, Ng *et al.*, 2007; Patil, Chantrapromma *et al.*, 2007).

In the molecular structure (Fig. 1), intramolecular C—H···O [H···O 2.41-2.46 Å, C···O 2.737 (4)-2.794 (4)Å and C—H···O 100-102°] and C—H···S [H···S 2.81-2.87 Å, C···S 3.171 (3)-3.190 (3) Å and C—H···S 103-104°] interactions generate S(5) ring motifs (Bernstein *et al.*, 1995). In the crystal structure, the molecules are linked into layers parallel to the [0 1 1] plane by intermolecular C—H···O hydrogen bonds (Fig. 2 and Table 1). In addition, short intermolecular Br···O contacts [2.997 (2) Å-3.110 (2) Å] are observed.

Experimental

An aqueous solution of NaOH (10%, 10 ml) was slowly added with stirring (4 h) to a solution 3-methylthiophene-2-carbaldehyde (0.01 mol) and 4-bromoacetophenone (0.01 mol) in methanol (60 ml). The reaction mixture was diluted with water (250 ml), and kept aside for 12 h. The resulting solid was collected by filtration, dried and recrystallized from acetone. Yellow block-shaped single crystals of (I) suitable for X-ray analysis were grown by slow evaporation of an acetone solution at room temperature.

Refinement

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H distances in the range 0.93–0.96 Å. The U_{iso} values were constrained to be $1.5U_{eq}$ of the carrier atom for methyl H atoms and $1.2U_{eq}$ for the remaining H atoms. A rotating group model was used for the methyl groups. The highest residual density peak is located 0.87 Å from atom Br1B and the deepest hole is located 0.89 Å from atom Br1C.

Figures

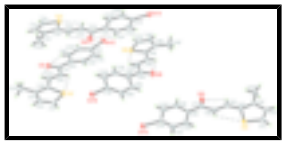

Fig. 1. The asymmetric unit of (I), showing 50% probability displacement ellipsoids and the atomic numbering. Dashed lines indicate hydrogen bonds.

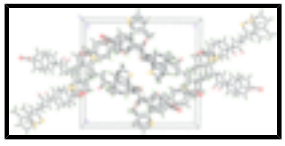

Fig. 2. The crystal packing of (I), viewed along the *a* axis. Hydrogen bonds are shown as dashed lines.

1-(4-Bromophenyl)-3-(3-methyl-2-thienyl)prop-2-en-1-one

Crystal data

$C_{14}H_{11}BrOS$	$Z = 8$
$M_r = 307.20$	$F_{000} = 1232$
Triclinic, $P\overline{1}$	$D_x = 1.647$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.4329$ (3) Å	Cell parameters from 14381 reflections
$b = 17.3541$ (7) Å	$\theta = 1.1$–30.0º
$c = 19.2551$ (8) Å	$\mu = 3.47$ mm^{-1}
$\alpha = 90.736$ (2)º	$T = 100.0$ (1) K
$\beta = 90.731$ (2)º	Block, yellow
$\gamma = 93.942$ (2)º	0.56 × 0.54 × 0.34 mm
$V = 2477.43$ (17) Å^3	

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer	14381 independent reflections
Radiation source: fine-focus sealed tube	10457 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.042$
Detector resolution: 8.33 pixels mm^{-1}	$\theta_{max} = 30.0$º
$T = 100.0(1)$ K	$\theta_{min} = 1.1$º
ω scans	$h = -10 \rightarrow 10$
Absorption correction: multi-scan (SADABS; Bruker, 2005)	$k = -24 \rightarrow 16$
$T_{min} = 0.165$, $T_{max} = 0.307$	$l = -27 \rightarrow 27$
42459 measured reflections	

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0562P)^2 + 0.0358P]$ where $P = (F_o^2 + 2F_c^2)/3$

$R[F^2 > 2\sigma(F^2)] = 0.038$

$wR(F^2) = 0.108$

$S = 1.06$

14381 reflections

617 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

$(\Delta/\sigma)_{max} = 0.002$

$\Delta\rho_{max} = 1.18$ e Å^{-3}

$\Delta\rho_{min} = -0.91$ e Å^{-3}

Extinction correction: none

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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	−0.10165 (4)	0.310304 (17)	−0.001640 (14)	0.02312 (7)
S1A	0.22066 (10)	0.02292 (4)	0.39343 (4)	0.02289 (15)
O1A	−0.0078 (3)	0.30625 (13)	0.34894 (11)	0.0365 (6)
C1A	0.2766 (4)	−0.02241 (17)	0.46806 (15)	0.0244 (6)
H1A	0.3248	−0.0704	0.4693	0.029*
C2A	0.2418 (4)	0.02041 (17)	0.52540 (15)	0.0239 (6)
H2A	0.2634	0.0043	0.5705	0.029*
C3A	0.1699 (4)	0.09143 (16)	0.51014 (14)	0.0210 (6)
C4A	0.1498 (4)	0.10185 (16)	0.43957 (15)	0.0222 (6)
C5A	0.0874 (4)	0.16816 (17)	0.40504 (15)	0.0238 (6)
H5A	0.0532	0.2082	0.4335	0.029*
C6A	0.0729 (4)	0.17880 (17)	0.33661 (16)	0.0249 (6)
H6A	0.0975	0.1392	0.3059	0.030*
C7A	0.0184 (4)	0.25267 (17)	0.30956 (16)	0.0256 (6)
C8A	−0.0036 (4)	0.26287 (17)	0.23283 (14)	0.0229 (6)
C9A	−0.0603 (4)	0.33339 (17)	0.21070 (16)	0.0259 (6)
H9A	−0.0794	0.3719	0.2433	0.031*
C10A	−0.0886 (4)	0.34700 (17)	0.14144 (16)	0.0254 (6)
H10A	−0.1261	0.3944	0.1272	0.031*
C11A	−0.0609 (4)	0.28962 (16)	0.09290 (14)	0.0204 (6)
C12A	−0.0034 (4)	0.21897 (17)	0.11279 (15)	0.0242 (6)
H12A	0.0159	0.1809	0.0798	0.029*

C13A	0.0250 (4)	0.20604 (18)	0.18297 (15)	0.0256 (6)
H13A	0.0636	0.1588	0.1970	0.031*
C14A	0.1198 (4)	0.14848 (17)	0.56469 (15)	0.0269 (6)
H14A	0.1440	0.2000	0.5480	0.040*
H14B	0.1896	0.1417	0.6062	0.040*
H14C	−0.0062	0.1401	0.5747	0.040*
Br1B	0.06425 (4)	0.641083 (17)	0.504583 (14)	0.02379 (7)
S1B	0.40741 (10)	0.35868 (4)	0.11048 (4)	0.02231 (15)
O1B	0.1524 (3)	0.63852 (12)	0.15444 (11)	0.0319 (5)
C1B	0.4340 (4)	0.30589 (17)	0.03649 (15)	0.0241 (6)
H1B	0.4787	0.2571	0.0358	0.029*
C2B	0.3829 (4)	0.34293 (17)	−0.02093 (15)	0.0235 (6)
H2B	0.3894	0.3222	−0.0655	0.028*
C3B	0.3184 (4)	0.41623 (16)	−0.00688 (15)	0.0216 (6)
C4B	0.3227 (4)	0.43335 (16)	0.06360 (14)	0.0190 (5)
C5B	0.2649 (4)	0.50129 (16)	0.09745 (15)	0.0223 (6)
H5B	0.2291	0.5403	0.0688	0.027*
C6B	0.2571 (4)	0.51440 (16)	0.16581 (15)	0.0219 (6)
H6B	0.2932	0.4773	0.1965	0.026*
C7B	0.1921 (4)	0.58672 (16)	0.19313 (15)	0.0220 (6)
C8B	0.1702 (4)	0.59630 (16)	0.26971 (14)	0.0195 (5)
C9B	0.1477 (4)	0.67065 (16)	0.29517 (14)	0.0216 (6)
H9B	0.1522	0.7119	0.2648	0.026*
C10B	0.1189 (4)	0.68366 (17)	0.36492 (15)	0.0239 (6)
H10B	0.1051	0.7334	0.3815	0.029*
C11B	0.1107 (4)	0.62180 (17)	0.40995 (14)	0.0213 (6)
C12B	0.1358 (4)	0.54770 (17)	0.38653 (15)	0.0237 (6)
H12B	0.1320	0.5067	0.4173	0.028*
C13B	0.1668 (4)	0.53542 (16)	0.31644 (15)	0.0224 (6)
H13B	0.1857	0.4859	0.3004	0.027*
C14B	0.2471 (4)	0.46610 (18)	−0.06228 (15)	0.0276 (6)
H14D	0.2317	0.5166	−0.0434	0.041*
H14E	0.1330	0.4436	−0.0792	0.041*
H14F	0.3308	0.4700	−0.0998	0.041*
Br1C	0.53300 (4)	0.176342 (17)	0.183227 (14)	0.02309 (7)
S1C	0.34254 (10)	0.49116 (4)	0.58077 (4)	0.02323 (15)
O1C	0.5620 (3)	0.20584 (12)	0.53536 (10)	0.0259 (4)
C1C	0.2863 (4)	0.53832 (17)	0.65503 (15)	0.0254 (6)
H1C	0.2566	0.5895	0.6566	0.031*
C2C	0.2900 (4)	0.49220 (17)	0.71170 (15)	0.0246 (6)
H2C	0.2642	0.5088	0.7564	0.029*
C3C	0.3371 (4)	0.41634 (17)	0.69565 (15)	0.0232 (6)
C4C	0.3716 (4)	0.40718 (16)	0.62578 (15)	0.0198 (5)
C5C	0.4270 (4)	0.33909 (16)	0.59083 (14)	0.0204 (6)
H5C	0.4495	0.2976	0.6190	0.024*
C6C	0.4501 (4)	0.32831 (16)	0.52246 (14)	0.0199 (5)
H6C	0.4243	0.3670	0.4917	0.024*
C7C	0.5159 (4)	0.25586 (16)	0.49582 (14)	0.0203 (6)
C8C	0.5224 (4)	0.24214 (16)	0.41909 (14)	0.0194 (5)

C9C	0.5869 (4)	0.17268 (17)	0.39661 (15)	0.0264 (6)
H9C	0.6282	0.1386	0.4291	0.032*
C10C	0.5906 (4)	0.15367 (17)	0.32688 (15)	0.0256 (6)
H10C	0.6329	0.1069	0.3125	0.031*
C11C	0.5307 (4)	0.20483 (16)	0.27847 (14)	0.0208 (6)
C12C	0.4694 (4)	0.27475 (16)	0.29928 (15)	0.0242 (6)
H12C	0.4318	0.3093	0.2665	0.029*
C13C	0.4644 (4)	0.29274 (16)	0.36920 (14)	0.0216 (6)
H13C	0.4216	0.3395	0.3833	0.026*
C14C	0.3428 (4)	0.35462 (18)	0.74890 (15)	0.0278 (7)
H14G	0.3778	0.3079	0.7274	0.042*
H14H	0.2256	0.3456	0.7688	0.042*
H14I	0.4287	0.3708	0.7848	0.042*
Br1D	0.43088 (4)	0.857276 (17)	0.320365 (14)	0.02597 (8)
S1D	0.12610 (10)	1.14678 (4)	−0.07243 (4)	0.02260 (15)
O1D	0.3873 (3)	0.86904 (12)	−0.03190 (10)	0.0272 (5)
C1D	0.0671 (4)	1.19363 (17)	−0.14590 (15)	0.0253 (6)
H1D	0.0313	1.2439	−0.1464	0.030*
C2D	0.0791 (4)	1.14818 (17)	−0.20368 (15)	0.0233 (6)
H2D	0.0525	1.1644	−0.2483	0.028*
C3D	0.1359 (4)	1.07380 (16)	−0.18900 (14)	0.0210 (6)
C4D	0.1677 (4)	1.06394 (16)	−0.11917 (14)	0.0190 (5)
C5D	0.2316 (4)	0.99729 (16)	−0.08575 (14)	0.0185 (5)
H5D	0.2602	0.9567	−0.1146	0.022*
C6D	0.2543 (4)	0.98747 (16)	−0.01763 (14)	0.0194 (5)
H6D	0.2193	1.0247	0.0136	0.023*
C7D	0.3352 (4)	0.91752 (16)	0.00857 (14)	0.0197 (5)
C8D	0.3539 (3)	0.90640 (16)	0.08476 (14)	0.0182 (5)
C9D	0.3961 (4)	0.83388 (16)	0.10723 (15)	0.0211 (6)
H9D	0.4086	0.7945	0.0748	0.025*
C10D	0.4196 (4)	0.81935 (17)	0.17707 (15)	0.0228 (6)
H10D	0.4465	0.7706	0.1917	0.027*
C11D	0.4025 (4)	0.87879 (17)	0.22492 (14)	0.0214 (6)
C12D	0.3609 (4)	0.95176 (17)	0.20408 (15)	0.0236 (6)
H12D	0.3494	0.9910	0.2367	0.028*
C13D	0.3366 (4)	0.96525 (16)	0.13381 (14)	0.0206 (6)
H13D	0.3086	1.0139	0.1193	0.025*
C14D	0.1559 (4)	1.01363 (17)	−0.24453 (14)	0.0263 (6)
H14L	0.1864	0.9663	−0.2235	0.039*
H14J	0.2498	1.0311	−0.2755	0.039*
H14K	0.0444	1.0050	−0.2700	0.039*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1A	0.02638 (14)	0.02635 (15)	0.01676 (14)	0.00262 (11)	−0.00219 (11)	0.00349 (11)
S1A	0.0299 (4)	0.0222 (3)	0.0168 (3)	0.0037 (3)	−0.0015 (3)	0.0019 (3)
O1A	0.0639 (16)	0.0296 (12)	0.0177 (11)	0.0158 (11)	−0.0010 (11)	0.0001 (9)

C1A	0.0302 (15)	0.0221 (14)	0.0215 (15)	0.0062 (12)	−0.0017 (12)	0.0047 (11)
C2A	0.0289 (15)	0.0262 (15)	0.0165 (14)	0.0014 (12)	−0.0041 (11)	0.0047 (11)
C3A	0.0217 (13)	0.0226 (14)	0.0188 (14)	0.0031 (11)	−0.0030 (11)	0.0014 (11)
C4A	0.0242 (14)	0.0218 (14)	0.0204 (14)	0.0007 (11)	0.0006 (11)	0.0025 (11)
C5A	0.0277 (15)	0.0224 (14)	0.0216 (15)	0.0042 (11)	−0.0044 (12)	0.0010 (11)
C6A	0.0300 (15)	0.0212 (14)	0.0235 (15)	0.0021 (12)	−0.0017 (12)	0.0043 (11)
C7A	0.0300 (15)	0.0257 (15)	0.0214 (15)	0.0041 (12)	−0.0008 (12)	0.0044 (12)
C8A	0.0246 (14)	0.0284 (15)	0.0153 (13)	0.0002 (12)	−0.0018 (11)	0.0013 (11)
C9A	0.0322 (16)	0.0226 (14)	0.0233 (15)	0.0048 (12)	0.0019 (12)	−0.0010 (12)
C10A	0.0300 (15)	0.0228 (15)	0.0244 (15)	0.0080 (12)	−0.0014 (12)	0.0047 (12)
C11A	0.0206 (13)	0.0229 (14)	0.0175 (13)	0.0012 (11)	−0.0004 (10)	0.0015 (11)
C12A	0.0292 (15)	0.0238 (15)	0.0196 (14)	0.0024 (12)	0.0008 (12)	0.0004 (11)
C13A	0.0310 (16)	0.0267 (15)	0.0194 (14)	0.0049 (12)	−0.0009 (12)	0.0031 (12)
C14A	0.0356 (16)	0.0253 (15)	0.0203 (15)	0.0064 (13)	−0.0007 (12)	0.0024 (12)
Br1B	0.02915 (15)	0.02746 (15)	0.01495 (13)	0.00330 (11)	−0.00046 (11)	0.00104 (11)
S1B	0.0277 (4)	0.0219 (3)	0.0177 (3)	0.0055 (3)	−0.0017 (3)	0.0024 (3)
O1B	0.0522 (14)	0.0242 (11)	0.0206 (11)	0.0120 (10)	−0.0044 (10)	0.0010 (9)
C1B	0.0242 (14)	0.0248 (15)	0.0239 (15)	0.0066 (11)	0.0011 (12)	0.0019 (12)
C2B	0.0272 (14)	0.0269 (15)	0.0172 (14)	0.0080 (12)	−0.0019 (11)	−0.0021 (11)
C3B	0.0235 (14)	0.0228 (14)	0.0186 (14)	0.0030 (11)	−0.0022 (11)	0.0000 (11)
C4B	0.0208 (13)	0.0193 (13)	0.0172 (13)	0.0030 (10)	−0.0038 (10)	0.0031 (10)
C5B	0.0223 (14)	0.0192 (14)	0.0257 (15)	0.0035 (11)	−0.0035 (11)	0.0021 (11)
C6B	0.0286 (15)	0.0196 (14)	0.0181 (14)	0.0056 (11)	−0.0024 (11)	0.0013 (11)
C7B	0.0262 (14)	0.0199 (14)	0.0198 (14)	0.0020 (11)	−0.0027 (11)	−0.0001 (11)
C8B	0.0200 (13)	0.0214 (14)	0.0175 (13)	0.0048 (10)	−0.0044 (10)	0.0020 (11)
C9B	0.0244 (14)	0.0220 (14)	0.0185 (14)	0.0029 (11)	−0.0029 (11)	0.0028 (11)
C10B	0.0292 (15)	0.0216 (14)	0.0211 (15)	0.0031 (11)	−0.0002 (12)	−0.0008 (11)
C11B	0.0242 (14)	0.0266 (15)	0.0126 (13)	−0.0015 (11)	−0.0009 (10)	−0.0003 (11)
C12B	0.0289 (15)	0.0233 (14)	0.0189 (14)	0.0019 (12)	−0.0040 (12)	0.0028 (11)
C13B	0.0293 (15)	0.0184 (13)	0.0199 (14)	0.0039 (11)	−0.0046 (11)	0.0015 (11)
C14B	0.0342 (16)	0.0283 (16)	0.0209 (15)	0.0079 (13)	−0.0043 (12)	0.0026 (12)
Br1C	0.03045 (15)	0.02499 (15)	0.01402 (13)	0.00372 (11)	−0.00169 (11)	−0.00025 (10)
S1C	0.0313 (4)	0.0205 (3)	0.0183 (3)	0.0029 (3)	0.0027 (3)	0.0027 (3)
O1C	0.0387 (12)	0.0236 (11)	0.0163 (10)	0.0097 (9)	−0.0019 (9)	0.0033 (8)
C1C	0.0303 (15)	0.0224 (15)	0.0239 (15)	0.0038 (12)	0.0034 (12)	−0.0017 (12)
C2C	0.0277 (15)	0.0260 (15)	0.0202 (14)	0.0039 (12)	−0.0002 (12)	−0.0021 (11)
C3C	0.0237 (14)	0.0253 (15)	0.0205 (14)	−0.0003 (11)	−0.0020 (11)	0.0025 (11)
C4C	0.0196 (13)	0.0198 (13)	0.0197 (14)	0.0009 (10)	−0.0033 (10)	0.0022 (11)
C5C	0.0223 (13)	0.0213 (14)	0.0175 (13)	0.0017 (11)	−0.0044 (11)	0.0012 (11)
C6C	0.0256 (14)	0.0182 (13)	0.0163 (13)	0.0034 (11)	−0.0027 (11)	0.0024 (10)
C7C	0.0252 (14)	0.0199 (13)	0.0160 (13)	0.0028 (11)	−0.0011 (11)	−0.0007 (10)
C8C	0.0236 (13)	0.0209 (14)	0.0135 (13)	0.0007 (11)	−0.0016 (10)	−0.0004 (10)
C9C	0.0377 (17)	0.0262 (15)	0.0165 (14)	0.0117 (13)	−0.0034 (12)	0.0040 (11)
C10C	0.0365 (16)	0.0226 (15)	0.0194 (14)	0.0140 (12)	0.0002 (12)	−0.0021 (11)
C11C	0.0261 (14)	0.0217 (14)	0.0142 (13)	−0.0011 (11)	−0.0008 (11)	−0.0013 (10)
C12C	0.0337 (16)	0.0205 (14)	0.0184 (14)	0.0012 (12)	−0.0039 (12)	0.0029 (11)
C13C	0.0279 (14)	0.0194 (14)	0.0179 (14)	0.0054 (11)	−0.0035 (11)	0.0001 (11)
C14C	0.0345 (16)	0.0287 (16)	0.0211 (15)	0.0068 (13)	−0.0004 (13)	0.0043 (12)
Br1D	0.03986 (17)	0.02542 (15)	0.01309 (13)	0.00557 (12)	−0.00239 (12)	0.00274 (11)

S1D	0.0296 (4)	0.0216 (3)	0.0173 (3)	0.0064 (3)	0.0000 (3)	0.0010 (3)
O1D	0.0411 (12)	0.0249 (11)	0.0166 (10)	0.0105 (9)	−0.0026 (9)	−0.0012 (8)
C1D	0.0305 (15)	0.0238 (15)	0.0225 (15)	0.0061 (12)	0.0034 (12)	0.0037 (12)
C2D	0.0262 (14)	0.0261 (15)	0.0183 (14)	0.0053 (12)	−0.0030 (11)	0.0063 (11)
C3D	0.0216 (13)	0.0242 (14)	0.0172 (13)	0.0033 (11)	−0.0028 (11)	0.0002 (11)
C4D	0.0193 (13)	0.0213 (13)	0.0165 (13)	0.0027 (10)	−0.0015 (10)	0.0003 (10)
C5D	0.0207 (13)	0.0200 (13)	0.0151 (13)	0.0041 (10)	−0.0024 (10)	−0.0004 (10)
C6D	0.0220 (13)	0.0199 (13)	0.0169 (13)	0.0057 (10)	−0.0027 (10)	0.0003 (10)
C7D	0.0221 (13)	0.0188 (13)	0.0186 (14)	0.0033 (10)	−0.0007 (11)	0.0014 (10)
C8D	0.0172 (12)	0.0232 (14)	0.0144 (13)	0.0024 (10)	−0.0027 (10)	0.0022 (10)
C9D	0.0253 (14)	0.0202 (14)	0.0181 (14)	0.0045 (11)	−0.0022 (11)	−0.0011 (11)
C10D	0.0292 (15)	0.0194 (14)	0.0202 (14)	0.0040 (11)	−0.0011 (12)	0.0027 (11)
C11D	0.0241 (14)	0.0255 (14)	0.0147 (13)	0.0028 (11)	−0.0016 (11)	0.0037 (11)
C12D	0.0302 (15)	0.0224 (14)	0.0184 (14)	0.0039 (12)	0.0000 (12)	−0.0002 (11)
C13D	0.0273 (14)	0.0192 (13)	0.0153 (13)	0.0032 (11)	−0.0018 (11)	−0.0006 (10)
C14D	0.0386 (17)	0.0251 (15)	0.0151 (14)	0.0032 (13)	−0.0083 (12)	−0.0003 (11)

Geometric parameters (Å, °)

Br1A—C11A	1.885 (3)	Br1C—C11C	1.894 (3)
S1A—C1A	1.707 (3)	S1C—C1C	1.709 (3)
S1A—C4A	1.739 (3)	S1C—C4C	1.730 (3)
O1A—C7A	1.220 (4)	O1C—C7C	1.225 (3)
C1A—C2A	1.360 (4)	C1C—C2C	1.363 (4)
C1A—H1A	0.93	C1C—H1C	0.93
C2A—C3A	1.410 (4)	C2C—C3C	1.417 (4)
C2A—H2A	0.93	C2C—H2C	0.93
C3A—C4A	1.381 (4)	C3C—C4C	1.382 (4)
C3A—C14A	1.502 (4)	C3C—C14C	1.495 (4)
C4A—C5A	1.438 (4)	C4C—C5C	1.440 (4)
C5A—C6A	1.337 (4)	C5C—C6C	1.342 (4)
C5A—H5A	0.93	C5C—H5C	0.93
C6A—C7A	1.470 (4)	C6C—C7C	1.469 (4)
C6A—H6A	0.93	C6C—H6C	0.93
C7A—C8A	1.499 (4)	C7C—C8C	1.495 (4)
C8A—C9A	1.392 (4)	C8C—C9C	1.394 (4)
C8A—C13A	1.396 (4)	C8C—C13C	1.394 (4)
C9A—C10A	1.374 (4)	C9C—C10C	1.380 (4)
C9A—H9A	0.93	C9C—H9C	0.93
C10A—C11A	1.384 (4)	C10C—C11C	1.386 (4)
C10A—H10A	0.93	C10C—H10C	0.93
C11A—C12A	1.383 (4)	C11C—C12C	1.382 (4)
C12A—C13A	1.388 (4)	C12C—C13C	1.380 (4)
C12A—H12A	0.93	C12C—H12C	0.93
C13A—H13A	0.93	C13C—H13C	0.93
C14A—H14A	0.96	C14C—H14G	0.96
C14A—H14B	0.96	C14C—H14H	0.96
C14A—H14C	0.96	C14C—H14I	0.96
Br1B—C11B	1.889 (3)	Br1D—C11D	1.892 (3)

S1B—C1B	1.705 (3)	S1D—C1D	1.708 (3)
S1B—C4B	1.737 (3)	S1D—C4D	1.734 (3)
O1B—C7B	1.224 (3)	O1D—C7D	1.225 (3)
C1B—C2B	1.349 (4)	C1D—C2D	1.363 (4)
C1B—H1B	0.93	C1D—H1D	0.93
C2B—C3B	1.414 (4)	C2D—C3D	1.416 (4)
C2B—H2B	0.93	C2D—H2D	0.93
C3B—C4B	1.385 (4)	C3D—C4D	1.377 (4)
C3B—C14B	1.497 (4)	C3D—C14D	1.501 (4)
C4B—C5B	1.434 (4)	C4D—C5D	1.437 (4)
C5B—C6B	1.336 (4)	C5D—C6D	1.335 (4)
C5B—H5B	0.93	C5D—H5D	0.93
C6B—C7B	1.469 (4)	C6D—C7D	1.482 (4)
C6B—H6B	0.93	C6D—H6D	0.93
C7B—C8B	1.494 (4)	C7D—C8D	1.488 (4)
C8B—C13B	1.396 (4)	C8D—C9D	1.391 (4)
C8B—C9B	1.396 (4)	C8D—C13D	1.396 (4)
C9B—C10B	1.381 (4)	C9D—C10D	1.383 (4)
C9B—H9B	0.93	C9D—H9D	0.93
C10B—C11B	1.387 (4)	C10D—C11D	1.388 (4)
C10B—H10B	0.93	C10D—H10D	0.93
C11B—C12B	1.383 (4)	C11D—C12D	1.387 (4)
C12B—C13B	1.388 (4)	C12D—C13D	1.388 (4)
C12B—H12B	0.93	C12D—H12D	0.93
C13B—H13B	0.93	C13D—H13D	0.93
C14B—H14D	0.96	C14D—H14L	0.96
C14B—H14E	0.96	C14D—H14J	0.96
C14B—H14F	0.96	C14D—H14K	0.96
C1A—S1A—C4A	91.91 (14)	C1C—S1C—C4C	91.55 (14)
C2A—C1A—S1A	111.6 (2)	C2C—C1C—S1C	112.1 (2)
C2A—C1A—H1A	124.2	C2C—C1C—H1C	123.9
S1A—C1A—H1A	124.2	S1C—C1C—H1C	123.9
C1A—C2A—C3A	113.7 (3)	C1C—C2C—C3C	113.1 (3)
C1A—C2A—H2A	123.2	C1C—C2C—H2C	123.4
C3A—C2A—H2A	123.2	C3C—C2C—H2C	123.4
C4A—C3A—C2A	112.2 (3)	C4C—C3C—C2C	111.8 (3)
C4A—C3A—C14A	124.3 (3)	C4C—C3C—C14C	125.5 (3)
C2A—C3A—C14A	123.6 (3)	C2C—C3C—C14C	122.8 (3)
C3A—C4A—C5A	127.6 (3)	C3C—C4C—C5C	127.5 (3)
C3A—C4A—S1A	110.6 (2)	C3C—C4C—S1C	111.4 (2)
C5A—C4A—S1A	121.7 (2)	C5C—C4C—S1C	121.0 (2)
C6A—C5A—C4A	127.3 (3)	C6C—C5C—C4C	127.8 (3)
C6A—C5A—H5A	116.3	C6C—C5C—H5C	116.1
C4A—C5A—H5A	116.3	C4C—C5C—H5C	116.1
C5A—C6A—C7A	120.5 (3)	C5C—C6C—C7C	120.6 (2)
C5A—C6A—H6A	119.8	C5C—C6C—H6C	119.7
C7A—C6A—H6A	119.8	C7C—C6C—H6C	119.7
O1A—C7A—C6A	120.7 (3)	O1C—C7C—C6C	121.2 (2)
O1A—C7A—C8A	119.4 (3)	O1C—C7C—C8C	119.5 (2)

C6A—C7A—C8A	119.9 (3)	C6C—C7C—C8C	119.4 (2)
C9A—C8A—C13A	118.5 (3)	C9C—C8C—C13C	118.3 (3)
C9A—C8A—C7A	117.1 (3)	C9C—C8C—C7C	117.0 (2)
C13A—C8A—C7A	124.4 (3)	C13C—C8C—C7C	124.7 (3)
C10A—C9A—C8A	121.0 (3)	C10C—C9C—C8C	121.0 (3)
C10A—C9A—H9A	119.5	C10C—C9C—H9C	119.5
C8A—C9A—H9A	119.5	C8C—C9C—H9C	119.5
C9A—C10A—C11A	119.5 (3)	C9C—C10C—C11C	119.4 (3)
C9A—C10A—H10A	120.2	C9C—C10C—H10C	120.3
C11A—C10A—H10A	120.2	C11C—C10C—H10C	120.3
C12A—C11A—C10A	121.2 (3)	C12C—C11C—C10C	120.7 (3)
C12A—C11A—Br1A	120.5 (2)	C12C—C11C—Br1C	120.8 (2)
C10A—C11A—Br1A	118.3 (2)	C10C—C11C—Br1C	118.5 (2)
C11A—C12A—C13A	118.7 (3)	C13C—C12C—C11C	119.3 (3)
C11A—C12A—H12A	120.7	C13C—C12C—H12C	120.3
C13A—C12A—H12A	120.7	C11C—C12C—H12C	120.3
C12A—C13A—C8A	121.1 (3)	C12C—C13C—C8C	121.2 (3)
C12A—C13A—H13A	119.5	C12C—C13C—H13C	119.4
C8A—C13A—H13A	119.5	C8C—C13C—H13C	119.4
C3A—C14A—H14A	109.5	C3C—C14C—H14G	109.5
C3A—C14A—H14B	109.5	C3C—C14C—H14H	109.5
H14A—C14A—H14B	109.5	H14G—C14C—H14H	109.5
C3A—C14A—H14C	109.5	C3C—C14C—H14I	109.5
H14A—C14A—H14C	109.5	H14G—C14C—H14I	109.5
H14B—C14A—H14C	109.5	H14H—C14C—H14I	109.5
C1B—S1B—C4B	91.52 (14)	C1D—S1D—C4D	92.09 (14)
C2B—C1B—S1B	112.3 (2)	C2D—C1D—S1D	111.6 (2)
C2B—C1B—H1B	123.8	C2D—C1D—H1D	124.2
S1B—C1B—H1B	123.8	S1D—C1D—H1D	124.2
C1B—C2B—C3B	113.6 (3)	C1D—C2D—C3D	113.3 (3)
C1B—C2B—H2B	123.2	C1D—C2D—H2D	123.4
C3B—C2B—H2B	123.2	C3D—C2D—H2D	123.4
C4B—C3B—C2B	111.6 (2)	C4D—C3D—C2D	112.3 (3)
C4B—C3B—C14B	125.4 (3)	C4D—C3D—C14D	125.1 (3)
C2B—C3B—C14B	122.9 (3)	C2D—C3D—C14D	122.5 (3)
C3B—C4B—C5B	127.6 (3)	C3D—C4D—C5D	127.7 (3)
C3B—C4B—S1B	110.9 (2)	C3D—C4D—S1D	110.7 (2)
C5B—C4B—S1B	121.5 (2)	C5D—C4D—S1D	121.5 (2)
C6B—C5B—C4B	126.8 (3)	C6D—C5D—C4D	126.9 (3)
C6B—C5B—H5B	116.6	C6D—C5D—H5D	116.5
C4B—C5B—H5B	116.6	C4D—C5D—H5D	116.5
C5B—C6B—C7B	120.8 (3)	C5D—C6D—C7D	120.4 (3)
C5B—C6B—H6B	119.6	C5D—C6D—H6D	119.8
C7B—C6B—H6B	119.6	C7D—C6D—H6D	119.8
O1B—C7B—C6B	121.4 (3)	O1D—C7D—C6D	120.6 (3)
O1B—C7B—C8B	119.5 (3)	O1D—C7D—C8D	119.8 (2)
C6B—C7B—C8B	119.1 (2)	C6D—C7D—C8D	119.6 (2)
C13B—C8B—C9B	118.7 (3)	C9D—C8D—C13D	119.1 (3)
C13B—C8B—C7B	123.9 (3)	C9D—C8D—C7D	117.5 (3)

C9B—C8B—C7B	117.4 (2)	C13D—C8D—C7D	123.4 (2)
C10B—C9B—C8B	120.8 (3)	C10D—C9D—C8D	121.0 (3)
C10B—C9B—H9B	119.6	C10D—C9D—H9D	119.5
C8B—C9B—H9B	119.6	C8D—C9D—H9D	119.5
C9B—C10B—C11B	119.4 (3)	C9D—C10D—C11D	118.9 (3)
C9B—C10B—H10B	120.3	C9D—C10D—H10D	120.5
C11B—C10B—H10B	120.3	C11D—C10D—H10D	120.5
C12B—C11B—C10B	121.1 (3)	C12D—C11D—C10D	121.4 (3)
C12B—C11B—Br1B	120.5 (2)	C12D—C11D—Br1D	120.3 (2)
C10B—C11B—Br1B	118.4 (2)	C10D—C11D—Br1D	118.3 (2)
C11B—C12B—C13B	119.0 (3)	C11D—C12D—C13D	119.0 (3)
C11B—C12B—H12B	120.5	C11D—C12D—H12D	120.5
C13B—C12B—H12B	120.5	C13D—C12D—H12D	120.5
C12B—C13B—C8B	121.0 (3)	C12D—C13D—C8D	120.6 (3)
C12B—C13B—H13B	119.5	C12D—C13D—H13D	119.7
C8B—C13B—H13B	119.5	C8D—C13D—H13D	119.7
C3B—C14B—H14D	109.5	C3D—C14D—H14L	109.5
C3B—C14B—H14E	109.5	C3D—C14D—H14J	109.5
H14D—C14B—H14E	109.5	H14L—C14D—H14J	109.5
C3B—C14B—H14F	109.5	C3D—C14D—H14K	109.5
H14D—C14B—H14F	109.5	H14L—C14D—H14K	109.5
H14E—C14B—H14F	109.5	H14J—C14D—H14K	109.5
C4A—S1A—C1A—C2A	0.4 (2)	C4C—S1C—C1C—C2C	0.2 (2)
S1A—C1A—C2A—C3A	−0.4 (3)	S1C—C1C—C2C—C3C	−0.7 (3)
C1A—C2A—C3A—C4A	0.2 (4)	C1C—C2C—C3C—C4C	1.0 (4)
C1A—C2A—C3A—C14A	179.7 (3)	C1C—C2C—C3C—C14C	−177.5 (3)
C2A—C3A—C4A—C5A	−177.5 (3)	C2C—C3C—C4C—C5C	178.4 (3)
C14A—C3A—C4A—C5A	3.1 (5)	C14C—C3C—C4C—C5C	−3.0 (5)
C2A—C3A—C4A—S1A	0.0 (3)	C2C—C3C—C4C—S1C	−0.9 (3)
C14A—C3A—C4A—S1A	−179.4 (2)	C14C—C3C—C4C—S1C	177.7 (2)
C1A—S1A—C4A—C3A	−0.2 (2)	C1C—S1C—C4C—C3C	0.4 (2)
C1A—S1A—C4A—C5A	177.4 (2)	C1C—S1C—C4C—C5C	−179.0 (2)
C3A—C4A—C5A—C6A	178.0 (3)	C3C—C4C—C5C—C6C	175.6 (3)
S1A—C4A—C5A—C6A	0.7 (4)	S1C—C4C—C5C—C6C	−5.2 (4)
C4A—C5A—C6A—C7A	−175.7 (3)	C4C—C5C—C6C—C7C	177.1 (3)
C5A—C6A—C7A—O1A	2.8 (5)	C5C—C6C—C7C—O1C	−4.7 (4)
C5A—C6A—C7A—C8A	−177.9 (3)	C5C—C6C—C7C—C8C	173.7 (3)
O1A—C7A—C8A—C9A	−2.4 (4)	O1C—C7C—C8C—C9C	−1.9 (4)
C6A—C7A—C8A—C9A	178.2 (3)	C6C—C7C—C8C—C9C	179.6 (3)
O1A—C7A—C8A—C13A	179.2 (3)	O1C—C7C—C8C—C13C	176.4 (3)
C6A—C7A—C8A—C13A	−0.2 (4)	C6C—C7C—C8C—C13C	−2.1 (4)
C13A—C8A—C9A—C10A	0.3 (4)	C13C—C8C—C9C—C10C	−1.2 (4)
C7A—C8A—C9A—C10A	−178.3 (3)	C7C—C8C—C9C—C10C	177.2 (3)
C8A—C9A—C10A—C11A	0.2 (5)	C8C—C9C—C10C—C11C	0.6 (5)
C9A—C10A—C11A—C12A	−0.7 (4)	C9C—C10C—C11C—C12C	0.7 (5)
C9A—C10A—C11A—Br1A	179.9 (2)	C9C—C10C—C11C—Br1C	−178.8 (2)
C10A—C11A—C12A—C13A	0.6 (4)	C10C—C11C—C12C—C13C	−1.4 (4)
Br1A—C11A—C12A—C13A	−180.0 (2)	Br1C—C11C—C12C—C13C	178.1 (2)
C11A—C12A—C13A—C8A	0.0 (4)	C11C—C12C—C13C—C8C	0.9 (4)

C9A—C8A—C13A—C12A	−0.4 (4)	C9C—C8C—C13C—C12C	0.4 (4)
C7A—C8A—C13A—C12A	178.0 (3)	C7C—C8C—C13C—C12C	−177.9 (3)
C4B—S1B—C1B—C2B	0.5 (2)	C4D—S1D—C1D—C2D	−0.2 (2)
S1B—C1B—C2B—C3B	−0.4 (3)	S1D—C1D—C2D—C3D	0.3 (3)
C1B—C2B—C3B—C4B	0.0 (4)	C1D—C2D—C3D—C4D	−0.3 (4)
C1B—C2B—C3B—C14B	−177.3 (3)	C1D—C2D—C3D—C14D	179.1 (3)
C2B—C3B—C4B—C5B	−178.6 (3)	C2D—C3D—C4D—C5D	−178.0 (3)
C14B—C3B—C4B—C5B	−1.3 (5)	C14D—C3D—C4D—C5D	2.6 (5)
C2B—C3B—C4B—S1B	0.3 (3)	C2D—C3D—C4D—S1D	0.2 (3)
C14B—C3B—C4B—S1B	177.6 (2)	C14D—C3D—C4D—S1D	−179.2 (2)
C1B—S1B—C4B—C3B	−0.4 (2)	C1D—S1D—C4D—C3D	0.0 (2)
C1B—S1B—C4B—C5B	178.6 (2)	C1D—S1D—C4D—C5D	178.3 (2)
C3B—C4B—C5B—C6B	174.5 (3)	C3D—C4D—C5D—C6D	−176.9 (3)
S1B—C4B—C5B—C6B	−4.4 (4)	S1D—C4D—C5D—C6D	5.1 (4)
C4B—C5B—C6B—C7B	−179.1 (3)	C4D—C5D—C6D—C7D	−175.2 (3)
C5B—C6B—C7B—O1B	−3.9 (4)	C5D—C6D—C7D—O1D	2.3 (4)
C5B—C6B—C7B—C8B	174.7 (3)	C5D—C6D—C7D—C8D	−178.0 (3)
O1B—C7B—C8B—C13B	163.1 (3)	O1D—C7D—C8D—C9D	−12.9 (4)
C6B—C7B—C8B—C13B	−15.5 (4)	C6D—C7D—C8D—C9D	167.4 (2)
O1B—C7B—C8B—C9B	−15.3 (4)	O1D—C7D—C8D—C13D	165.2 (3)
C6B—C7B—C8B—C9B	166.0 (3)	C6D—C7D—C8D—C13D	−14.5 (4)
C13B—C8B—C9B—C10B	−1.4 (4)	C13D—C8D—C9D—C10D	0.4 (4)
C7B—C8B—C9B—C10B	177.2 (3)	C7D—C8D—C9D—C10D	178.6 (3)
C8B—C9B—C10B—C11B	−0.6 (4)	C8D—C9D—C10D—C11D	−0.7 (4)
C9B—C10B—C11B—C12B	1.8 (4)	C9D—C10D—C11D—C12D	0.6 (4)
C9B—C10B—C11B—Br1B	−178.2 (2)	C9D—C10D—C11D—Br1D	178.9 (2)
C10B—C11B—C12B—C13B	−1.1 (4)	C10D—C11D—C12D—C13D	−0.2 (4)
Br1B—C11B—C12B—C13B	179.0 (2)	Br1D—C11D—C12D—C13D	−178.5 (2)
C11B—C12B—C13B—C8B	−0.9 (4)	C11D—C12D—C13D—C8D	−0.1 (4)
C9B—C8B—C13B—C12B	2.1 (4)	C9D—C8D—C13D—C12D	−0.1 (4)
C7B—C8B—C13B—C12B	−176.3 (3)	C7D—C8D—C13D—C12D	−178.1 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1A—H1A···O1C^{i}	0.93	2.55	3.478 (4)	175
C5A—H5A···O1A	0.93	2.43	2.773 (4)	102
C6A—H6A···S1A	0.93	2.84	3.190 (3)	104
C9A—H9A···O1A	0.93	2.41	2.737 (4)	100
C1B—H1B···O1D^{ii}	0.93	2.47	3.397 (4)	177
C5B—H5B···O1B	0.93	2.46	2.794 (4)	101
C6B—H6B···S1B	0.93	2.81	3.171 (3)	104
C5C—H5C···O1C	0.93	2.44	2.789 (3)	102
C6C—H6C···S1C	0.93	2.84	3.184 (3)	103
C9C—H9C···O1C	0.93	2.42	2.737 (3)	100
C1D—H1D···O1B^{iii}	0.93	2.54	3.440 (4)	164
C5D—H5D···O1D	0.93	2.44	2.784 (4)	102
C6D—H6D···S1D	0.93	2.82	3.174 (3)	104

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*; (iii) −*x*, −*y*+2, −*z*.

Fig. 1

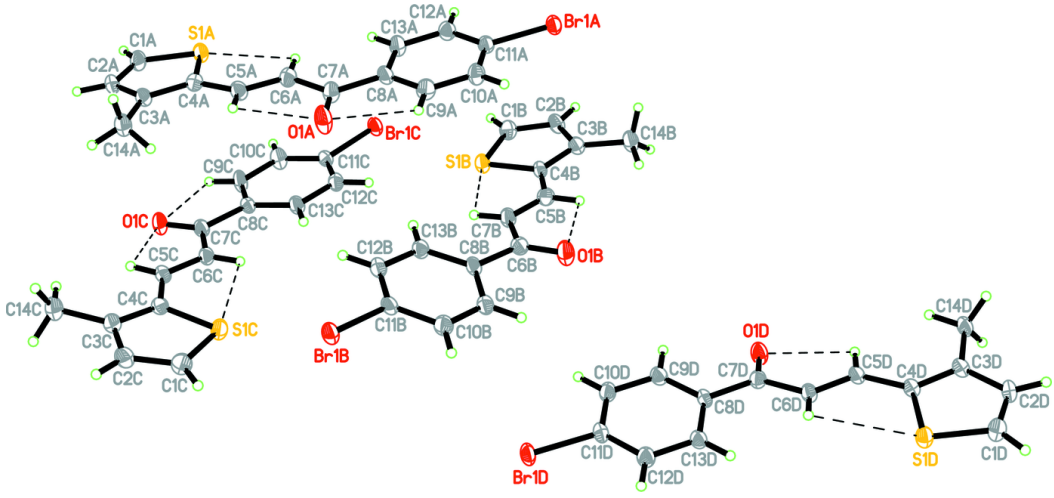

Fig. 2