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1,5-Bis(3-bromothien-2-yl)-3-(2,3,5-trichlorophenyl)pentane-1,5-dione

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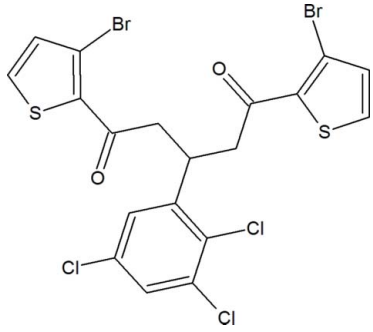
Key indicators: single-crystal X-ray study; T = 103 K; mean σ(C–C) = 0.003 Å; R factor = 0.030; wR factor = 0.073; data-to-parameter ratio = 23.9.

In the title compound, $C_{19}H_{11}Br_2Cl_3O_2S_2$, the angles between the plane of the 2,3,5-trichlorophenyl ring and those of the two 3-bromothien-2-yl rings are 89.7 (5) and 63.7 (1)°, with a dihedral angle of 77.4 (3)° between the last two planes.

Related literature

For general background, see: Tareen & Kutty (2001). For related literature on the title compound, see: Baxter *et al.* (1990); Ng *et al.* (2006); Yathirajan *et al.* (2006); Butcher *et al.* (2006*a*,*b*); Butcher, Yathirajan, Sarojini *et al.* (2006). For crystal structures of a series of related compounds, see: Baxter *et al.* (1990); Ng *et al.* (2006); Yathirajan *et al.* (2006).



Experimental

Crystal data

$C_{19}H_{11}Br_2Cl_3O_2S_2$
M_r = 601.57
Monoclinic, $P2_1/c$
a = 9.1380 (7) Å
b = 16.0009 (11) Å
c = 14.2139 (10) Å
β = 90.982 (1)°
V = 2078.0 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.50 mm^{-1}
T = 103 K
0.47 × 0.36 × 0.25 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.418, T_{max} = 1
(expected range = 0.136–0.324)
23415 measured reflections
6056 independent reflections
4876 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.073
S = 1.04
6056 reflections
253 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.62 e Å^{-3}

Data collection: *APEX2* (Bruker, 2006); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS86* (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: TK2165).

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supplementary materials

Acta Cryst. (2007). E**63**, o3330 [**doi:10.1107/S1600536807030589**]

1,5-Bis(3-bromothien-2-yl)-3-(2,3,5-trichlorophenyl)pentane-1,5-dione

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

Comment

The title compound, $C_{19}H_{11}Br_2Cl_3O_2S_2$, is a new derivative with potential in the high efficiency photovoltaic cell arena. Crystals of these types play an important role in electronic and photonic industries such as in the production of high efficiency photovoltaic cells, fabrication of bright and long-lasting light emitting diodes [LED] and in liquid crystal displays [LCD] (Tareen & Kutty, 2001). Present day demand is for large and high quality ferroelectric, piezoelectric single crystals with minimum defects and inhomogenities. In continuation of our work on crystal structures of new organic chalcones (Butcher *et al.*, 2006*a*; 2006*b*; Butcher, Yathirajan, Sarojini *et al.*, 2006), the title compound, (I), has been prepared and its crystal structure determined.

Molecules of (I) comprise two five-membered 3-bromothien-2-yl rings at each end of a pentane-1,5-dione group with a 2,3,5-trichlorophenyl ring at the 3-position. The angles between the plane of the 2,3,5-trichlorophenyl ring and the two 3-bromothien-2-yl rings are 89.7 (5)° and 63.7 (1)°, respectively, with a dihedral angle of 77.4 (3)° between the latter planes.

Experimental

2-Acetyl-3-bromothiophene (20 g, 0.096 mol) in methanol (50 ml) was mixed with 2,3,5-trichlorobenzaldehyde (9.84 g, 0.048 mol) and the mixture was treated with 30% potassium hydroxide solution (10 ml) at 278 K. The reaction mixture was then brought to room temperature and stirred for 6 h. The precipitate was filtered, washed with water, dried and recrytallized from acetone (yield 65%; m.p. 403–405 K). Elemental analysis found: C 37.81, H, 1.72, S, 10.54%; $C_{19}H_{11}Br_2Cl_3O_2S_2$ requires: C 37.93, H, 1.84, S, 10.66%.

Refinement

The H atoms were included in the riding model approximation with C—H = 0.95–1.00 Å, and with U_{iso}(H) = 1.17–1.28U_{eq}(C). The maximum residual electron density peaks of 1.11 and −0.62 e Å^{-3}, respectively, were located 0.26 and 0.31 Å from the Br1B and Cl3 atoms.

Figures

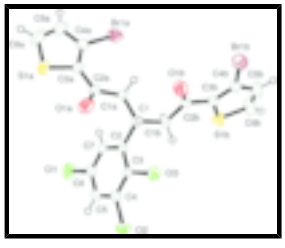


Fig. 1. Molecular structure of $C_{19}H_{11}Br_2Cl_3O_2S_2$, (I), showing atom labeling and 50% probability displacement ellipsoids.

1,5-Bis(3-bromothien-2-yl)-3-(2,3,5-trichlorophenyl)pentane-1,5-dione

Crystal data

$C_{19}H_{11}Br_2Cl_3O_2S_2$	F_{000} = 1176
M_r = 601.57	D_x = 1.923 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 8105 reflections
a = 9.1380 (7) Å	θ = 2.6–30.7º
b = 16.0009 (11) Å	μ = 4.50 mm^{-1}
c = 14.2139 (10) Å	T = 103 K
β = 90.982 (1)º	Block, colorless
V = 2078.0 (3) Å^3	0.47 × 0.36 × 0.25 mm
Z = 4	

Data collection

Bruker APEX2 CCD area-detector diffractometer	6056 independent reflections
Radiation source: fine-focus sealed tube	4876 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.049
Detector resolution: 0 pixels mm^{-1}	θ_{max} = 30.8º
T = 103 K	θ_{min} = 1.9º
φ and ω scans	h = −13→11
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	k = −21→22
T_{min} = 0.418, T_{max} = 1	l = −19→20
23415 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.030	H-atom parameters constrained
$wR(F^2)$ = 0.073	$w = 1/[\sigma^2(F_o^2) + (0.0387P)^2 + 0.0251P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max}$ = 0.002
6056 reflections	$\Delta\rho_{max}$ = 1.11 e Å^{-3}
253 parameters	$\Delta\rho_{min}$ = −0.62 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 $F^2 > 2\text{sigma}(F^2)$ 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	0.42307 (3)	0.511785 (13)	0.648516 (14)	0.01881 (6)
Br1B	1.12651 (2)	0.381058 (14)	0.725489 (16)	0.02260 (7)
Cl1	0.70399 (6)	0.05547 (3)	0.60137 (3)	0.01631 (10)
Cl2	0.49719 (6)	−0.09934 (3)	0.61154 (3)	0.01831 (11)
Cl3	0.04397 (6)	0.09993 (4)	0.69036 (4)	0.02140 (12)
S1A	0.21611 (7)	0.38361 (3)	0.40676 (4)	0.01961 (12)
S1B	0.83068 (6)	0.25216 (3)	0.91758 (3)	0.01789 (11)
O1A	0.41995 (19)	0.25982 (10)	0.47067 (11)	0.0240 (4)
O1B	0.83649 (17)	0.30796 (10)	0.64807 (10)	0.0211 (3)
C1	0.5688 (2)	0.22485 (12)	0.63890 (13)	0.0131 (4)
H1A	0.6381	0.2155	0.5862	0.016*
C2	0.4658 (2)	0.15015 (12)	0.64167 (13)	0.0127 (4)
C3	0.5207 (2)	0.06961 (12)	0.62640 (13)	0.0126 (4)
C4	0.4291 (2)	−0.00007 (12)	0.63045 (13)	0.0141 (4)
C5	0.2823 (2)	0.00884 (13)	0.64963 (14)	0.0161 (4)
H5A	0.2197	−0.0385	0.6523	0.019*
C6	0.2289 (2)	0.08842 (13)	0.66489 (14)	0.0148 (4)
C7	0.3180 (2)	0.15832 (13)	0.66149 (13)	0.0145 (4)
H7A	0.2779	0.2121	0.6727	0.017*
C1A	0.4946 (2)	0.30930 (12)	0.62241 (13)	0.0145 (4)
H1AA	0.4241	0.3193	0.6733	0.017*
H1AB	0.5697	0.3539	0.6261	0.017*
C2A	0.4146 (2)	0.31545 (13)	0.52842 (14)	0.0151 (4)
C3A	0.3280 (2)	0.39106 (13)	0.50608 (13)	0.0147 (4)
C4A	0.3183 (2)	0.47060 (13)	0.54265 (14)	0.0163 (4)
C5A	0.2239 (3)	0.52417 (14)	0.49206 (15)	0.0224 (5)
H5AA	0.2060	0.5808	0.5085	0.027*
C6A	0.1615 (3)	0.48482 (15)	0.41672 (17)	0.0247 (5)
H6AA	0.0945	0.5110	0.3742	0.030*
C1B	0.6602 (2)	0.22759 (13)	0.73140 (13)	0.0143 (4)
H1BA	0.5994	0.2513	0.7819	0.017*
H1BB	0.6870	0.1698	0.7498	0.017*
C2B	0.7981 (2)	0.27905 (13)	0.72335 (14)	0.0150 (4)

C3B	0.8870 (2)	0.29115 (13)	0.80966 (14)	0.0149 (4)
C4B	1.0196 (2)	0.33041 (13)	0.82200 (15)	0.0174 (4)
C5B	1.0748 (3)	0.32997 (14)	0.91510 (16)	0.0216 (5)
H5BA	1.1645	0.3553	0.9342	0.026*
C6B	0.9842 (3)	0.28887 (15)	0.97444 (16)	0.0236 (5)
H6BA	1.0039	0.2815	1.0397	0.028*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1A	0.02604 (13)	0.01413 (10)	0.01631 (10)	−0.00164 (8)	0.00192 (8)	−0.00241 (8)
Br1B	0.01341 (12)	0.02203 (12)	0.03247 (12)	−0.00257 (9)	0.00378 (9)	0.00598 (9)
Cl1	0.0119 (2)	0.0159 (2)	0.0212 (2)	0.00163 (19)	0.00085 (17)	−0.00031 (19)
Cl2	0.0222 (3)	0.0106 (2)	0.0221 (2)	0.00047 (19)	−0.00084 (19)	−0.00063 (18)
Cl3	0.0103 (3)	0.0265 (3)	0.0274 (3)	−0.0004 (2)	0.00133 (19)	0.0049 (2)
S1A	0.0215 (3)	0.0182 (3)	0.0190 (2)	0.0012 (2)	−0.0050 (2)	0.0011 (2)
S1B	0.0161 (3)	0.0215 (3)	0.0161 (2)	−0.0018 (2)	0.00106 (18)	−0.0008 (2)
O1A	0.0350 (10)	0.0158 (7)	0.0209 (7)	0.0063 (7)	−0.0061 (7)	−0.0054 (6)
O1B	0.0175 (9)	0.0255 (8)	0.0204 (7)	−0.0052 (7)	0.0004 (6)	0.0046 (6)
C1	0.0133 (10)	0.0112 (9)	0.0148 (8)	−0.0010 (8)	−0.0004 (7)	0.0005 (7)
C2	0.0139 (10)	0.0125 (9)	0.0115 (8)	−0.0001 (8)	−0.0013 (7)	0.0021 (7)
C3	0.0100 (10)	0.0139 (9)	0.0138 (8)	−0.0003 (8)	−0.0011 (7)	0.0008 (7)
C4	0.0172 (11)	0.0102 (9)	0.0147 (9)	−0.0001 (8)	−0.0031 (7)	−0.0003 (7)
C5	0.0169 (11)	0.0152 (10)	0.0161 (9)	−0.0060 (8)	−0.0038 (8)	0.0017 (8)
C6	0.0079 (10)	0.0207 (10)	0.0157 (9)	−0.0002 (8)	−0.0006 (7)	0.0029 (8)
C7	0.0147 (11)	0.0135 (9)	0.0152 (9)	0.0013 (8)	−0.0005 (7)	0.0005 (8)
C1A	0.0151 (11)	0.0123 (9)	0.0159 (9)	0.0004 (8)	−0.0005 (7)	0.0010 (8)
C2A	0.0149 (11)	0.0133 (9)	0.0172 (9)	−0.0007 (8)	0.0006 (7)	0.0015 (8)
C3A	0.0141 (11)	0.0150 (9)	0.0150 (9)	−0.0017 (8)	0.0027 (7)	0.0029 (8)
C4A	0.0188 (11)	0.0156 (10)	0.0145 (9)	0.0000 (8)	0.0022 (7)	0.0009 (8)
C5A	0.0266 (13)	0.0172 (11)	0.0233 (10)	0.0065 (9)	0.0021 (9)	0.0012 (9)
C6A	0.0229 (13)	0.0224 (11)	0.0287 (11)	0.0076 (10)	−0.0026 (9)	0.0056 (10)
C1B	0.0124 (10)	0.0136 (9)	0.0169 (9)	−0.0014 (8)	−0.0002 (7)	0.0009 (8)
C2B	0.0121 (10)	0.0122 (9)	0.0208 (9)	0.0021 (8)	0.0003 (7)	−0.0004 (8)
C3B	0.0128 (11)	0.0140 (9)	0.0178 (9)	−0.0010 (8)	0.0021 (7)	−0.0024 (8)
C4B	0.0143 (11)	0.0156 (10)	0.0223 (10)	0.0006 (8)	0.0017 (8)	−0.0014 (8)
C5B	0.0157 (12)	0.0213 (11)	0.0276 (11)	−0.0024 (9)	−0.0037 (9)	−0.0046 (9)
C6B	0.0236 (13)	0.0282 (12)	0.0188 (9)	−0.0005 (10)	−0.0044 (8)	−0.0061 (9)

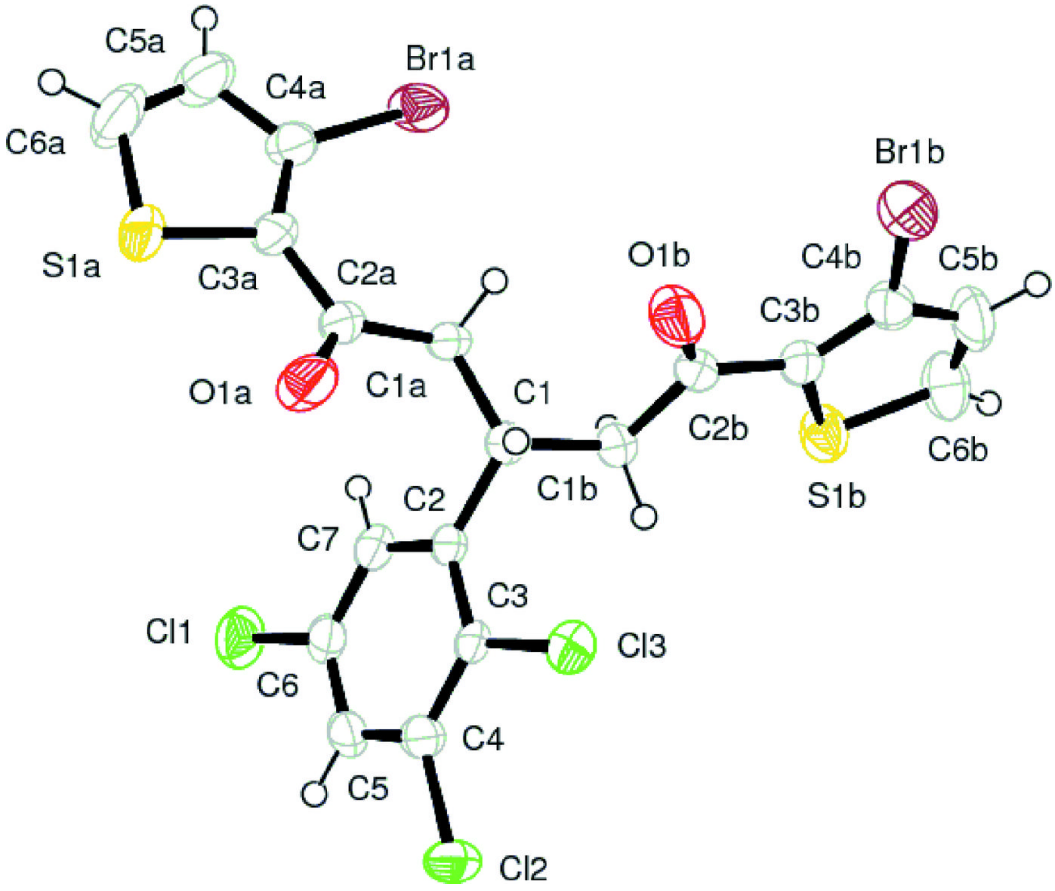
Geometric parameters (Å, °)

Br1A—C4A	1.888 (2)	C6—C7	1.385 (3)
Br1B—C4B	1.881 (2)	C7—H7A	0.9500
Cl1—C3	1.733 (2)	C1A—C2A	1.515 (3)
Cl2—C4	1.728 (2)	C1A—H1AA	0.9900
Cl3—C6	1.744 (2)	C1A—H1AB	0.9900
S1A—C6A	1.701 (2)	C2A—C3A	1.478 (3)
S1A—C3A	1.733 (2)	C3A—C4A	1.378 (3)
S1B—C6B	1.711 (2)	C4A—C5A	1.405 (3)

S1B—C3B	1.742 (2)	C5A—C6A	1.359 (3)
O1A—C2A	1.212 (2)	C5A—H5AA	0.9500
O1B—C2B	1.222 (2)	C6A—H6AA	0.9500
C1—C2	1.523 (3)	C1B—C2B	1.512 (3)
C1—C1A	1.528 (3)	C1B—H1BA	0.9900
C1—C1B	1.546 (3)	C1B—H1BB	0.9900
C1—H1A	1.0000	C2B—C3B	1.473 (3)
C2—C7	1.391 (3)	C3B—C4B	1.373 (3)
C2—C3	1.401 (3)	C4B—C5B	1.408 (3)
C3—C4	1.396 (3)	C5B—C6B	1.361 (3)
C4—C5	1.381 (3)	C5B—H5BA	0.9500
C5—C6	1.382 (3)	C6B—H6BA	0.9500
C5—H5A	0.9500		
C6A—S1A—C3A	92.10 (11)	C3A—C2A—C1A	119.43 (17)
C6B—S1B—C3B	92.33 (11)	C4A—C3A—C2A	135.45 (19)
C2—C1—C1A	115.15 (17)	C4A—C3A—S1A	109.28 (15)
C2—C1—C1B	108.98 (15)	C2A—C3A—S1A	115.17 (15)
C1A—C1—C1B	109.70 (16)	C3A—C4A—C5A	114.39 (19)
C2—C1—H1A	107.6	C3A—C4A—Br1A	126.02 (16)
C1A—C1—H1A	107.6	C5A—C4A—Br1A	119.55 (16)
C1B—C1—H1A	107.6	C6A—C5A—C4A	111.5 (2)
C7—C2—C3	118.00 (19)	C6A—C5A—H5AA	124.3
C7—C2—C1	122.32 (18)	C4A—C5A—H5AA	124.3
C3—C2—C1	119.65 (19)	C5A—C6A—S1A	112.74 (18)
C4—C3—C2	120.77 (19)	C5A—C6A—H6AA	123.6
C4—C3—Cl1	119.11 (16)	S1A—C6A—H6AA	123.6
C2—C3—Cl1	120.12 (16)	C2B—C1B—C1	112.93 (16)
C5—C4—C3	120.71 (19)	C2B—C1B—H1BA	109.0
C5—C4—Cl2	118.63 (16)	C1—C1B—H1BA	109.0
C3—C4—Cl2	120.66 (17)	C2B—C1B—H1BB	109.0
C4—C5—C6	118.25 (19)	C1—C1B—H1BB	109.0
C4—C5—H5A	120.9	H1BA—C1B—H1BB	107.8
C6—C5—H5A	120.9	O1B—C2B—C3B	121.1 (2)
C5—C6—C7	122.0 (2)	O1B—C2B—C1B	121.62 (18)
C5—C6—Cl3	118.43 (17)	C3B—C2B—C1B	117.21 (17)
C7—C6—Cl3	119.62 (17)	C4B—C3B—C2B	129.74 (19)
C6—C7—C2	120.31 (19)	C4B—C3B—S1B	108.96 (15)
C6—C7—H7A	119.8	C2B—C3B—S1B	121.30 (16)
C2—C7—H7A	119.8	C3B—C4B—C5B	114.8 (2)
C2A—C1A—C1	113.50 (16)	C3B—C4B—Br1B	124.89 (16)
C2A—C1A—H1AA	108.9	C5B—C4B—Br1B	120.35 (17)
C1—C1A—H1AA	108.9	C6B—C5B—C4B	111.9 (2)
C2A—C1A—H1AB	108.9	C6B—C5B—H5BA	124.1
C1—C1A—H1AB	108.9	C4B—C5B—H5BA	124.1
H1AA—C1A—H1AB	107.7	C5B—C6B—S1B	112.07 (17)
O1A—C2A—C3A	118.89 (18)	C5B—C6B—H6BA	124.0
O1A—C2A—C1A	121.68 (19)	S1B—C6B—H6BA	124.0
C1A—C1—C2—C7	−22.0 (3)	C6A—S1A—C3A—C4A	0.15 (17)

C1B—C1—C2—C7	101.8 (2)	C6A—S1A—C3A—C2A	−176.73 (17)
C1A—C1—C2—C3	159.82 (17)	C2A—C3A—C4A—C5A	175.8 (2)
C1B—C1—C2—C3	−76.4 (2)	S1A—C3A—C4A—C5A	−0.2 (2)
C7—C2—C3—C4	0.4 (3)	C2A—C3A—C4A—Br1A	−2.0 (4)
C1—C2—C3—C4	178.70 (17)	S1A—C3A—C4A—Br1A	−178.02 (12)
C7—C2—C3—Cl1	179.98 (14)	C3A—C4A—C5A—C6A	0.1 (3)
C1—C2—C3—Cl1	−1.7 (2)	Br1A—C4A—C5A—C6A	178.10 (17)
C2—C3—C4—C5	0.0 (3)	C4A—C5A—C6A—S1A	0.0 (3)
Cl1—C3—C4—C5	−179.60 (15)	C3A—S1A—C6A—C5A	−0.1 (2)
C2—C3—C4—Cl2	179.97 (14)	C2—C1—C1B—C2B	160.27 (17)
Cl1—C3—C4—Cl2	0.4 (2)	C1A—C1—C1B—C2B	−72.8 (2)
C3—C4—C5—C6	−0.2 (3)	C1—C1B—C2B—O1B	−6.3 (3)
Cl2—C4—C5—C6	179.84 (14)	C1—C1B—C2B—C3B	175.29 (17)
C4—C5—C6—C7	0.0 (3)	O1B—C2B—C3B—C4B	−2.4 (4)
C4—C5—C6—Cl3	−179.34 (15)	C1B—C2B—C3B—C4B	176.0 (2)
C5—C6—C7—C2	0.4 (3)	O1B—C2B—C3B—S1B	178.49 (17)
Cl3—C6—C7—C2	179.73 (14)	C1B—C2B—C3B—S1B	−3.1 (3)
C3—C2—C7—C6	−0.6 (3)	C6B—S1B—C3B—C4B	−0.16 (17)
C1—C2—C7—C6	−178.85 (17)	C6B—S1B—C3B—C2B	179.10 (18)
C2—C1—C1A—C2A	−62.4 (2)	C2B—C3B—C4B—C5B	−179.5 (2)
C1B—C1—C1A—C2A	174.27 (17)	S1B—C3B—C4B—C5B	−0.3 (2)
C1—C1A—C2A—O1A	−4.9 (3)	C2B—C3B—C4B—Br1B	−0.2 (3)
C1—C1A—C2A—C3A	175.17 (18)	S1B—C3B—C4B—Br1B	178.98 (12)
O1A—C2A—C3A—C4A	−164.8 (2)	C3B—C4B—C5B—C6B	0.8 (3)
C1A—C2A—C3A—C4A	15.1 (4)	Br1B—C4B—C5B—C6B	−178.53 (17)
O1A—C2A—C3A—S1A	11.0 (3)	C4B—C5B—C6B—S1B	−0.9 (3)
C1A—C2A—C3A—S1A	−169.05 (15)	C3B—S1B—C6B—C5B	0.6 (2)

Fig. 1


C5a
Br1a
C4a
C6a
Br1b
S1a
C3a
C2a
O1b
C4b
C5b
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C1a
C1
C2b
C6b
C1b
S1b
C2
C7
C3
Cl1
Cl3
C6
C4
C5
Cl2