



ISSN 1600-5368



# Crystal structure of 3-(2-bromophenyl-sulfonyl)-2,5,7-trimethyl-1-benzofuran

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Received 29 September 2014; accepted 3 October 2014

Edited by J. T. Mague, Tulane University, USA

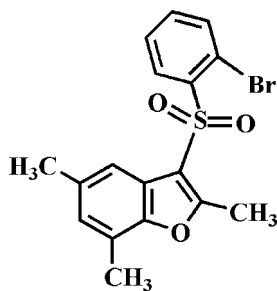
In the title compound, C<sub>17</sub>H<sub>15</sub>BrO<sub>3</sub>S, the dihedral angle between the planes of the benzofuran ring system [r.m.s. deviation = 0.016 (2) Å] and the 2-bromophenyl ring is 82.93 (6)°. In the crystal, molecules are linked *via* pairs of C—H···π hydrogen bonds and π–π interactions between the benzene and furan rings of neighbouring molecules [centroid–centroid distance = 3.881 (2) Å] into inversion-related dimers along the *b*-axis direction. These dimers are further linked by short Br···O [3.185 (2) Å] contacts.

**Keywords:** crystal structure; benzofuran; 2-bromophenyl; C—H···π hydrogen bonds; π–π interactions; Br···O contact.

**CCDC reference:** 1027593

## 1. Related literature

For a related structure and background to benzofuran derivatives, see: Choi & Lee (2014). For further synthetic details, see: Choi *et al.* (1999). For a review of halogen bonding, see: Politzer *et al.* (2007).



## 2. Experimental

### 2.1. Crystal data

C<sub>17</sub>H<sub>15</sub>BrO<sub>3</sub>S  
*M<sub>r</sub>* = 379.26  
 Monoclinic, *P*2<sub>1</sub>/*n*  
*a* = 7.8969 (2) Å  
*b* = 8.1489 (2) Å  
*c* = 24.3146 (6) Å  
 $\beta$  = 96.210 (1)°  
*V* = 1555.49 (7) Å<sup>3</sup>  
*Z* = 4  
 Mo *K*α radiation  
 $\mu$  = 2.79 mm<sup>-1</sup>  
*T* = 173 K  
 0.31 × 0.27 × 0.13 mm

### 2.2. Data collection

Bruker SMART APEXII CCD diffractometer  
 Absorption correction: multi-scan (*SADABS*; Bruker, 2009)  
*T*<sub>min</sub> = 0.479, *T*<sub>max</sub> = 0.713  
 27395 measured reflections  
 3867 independent reflections  
 3130 reflections with *I* > 2σ(*I*)  
*R*<sub>int</sub> = 0.042

### 2.3. Refinement

*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.031  
*wR*(*F*<sup>2</sup>) = 0.080  
*S* = 1.03  
 3867 reflections  
 202 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\max}$  = 0.51 e Å<sup>-3</sup>  
 $\Delta\rho_{\min}$  = -0.34 e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

Cg1 is the centroid of the C2–C7 benzene ring.

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C9—H9C···Cg1 <sup>1</sup>	0.98	2.84	3.608 (2)	136

Symmetry code: (i)  $-x + 1, -y + 1, -z + 1$ .

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* for Windows (Farrugia, 2012) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXL97*.

## Acknowledgements

The X-ray centre of Gyeongsang National University is acknowledged for providing access to the single-crystal diffractometer.

Supporting information for this paper is available from the IUCr electronic archives (Reference: MW2127).

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## supporting information

*Acta Cryst.* (2014). E70, o1152 [doi:10.1107/S1600536814021850]

## Crystal structure of 3-(2-bromophenylsulfonyl)-2,5,7-trimethyl-1-benzofuran

Hong Dae Choi and Uk Lee

### S1. Comment

As a part of our continuing program for benzofuran derivatives (Choi & Lee, 2014), we report herein on the crystal structure of the title compound.

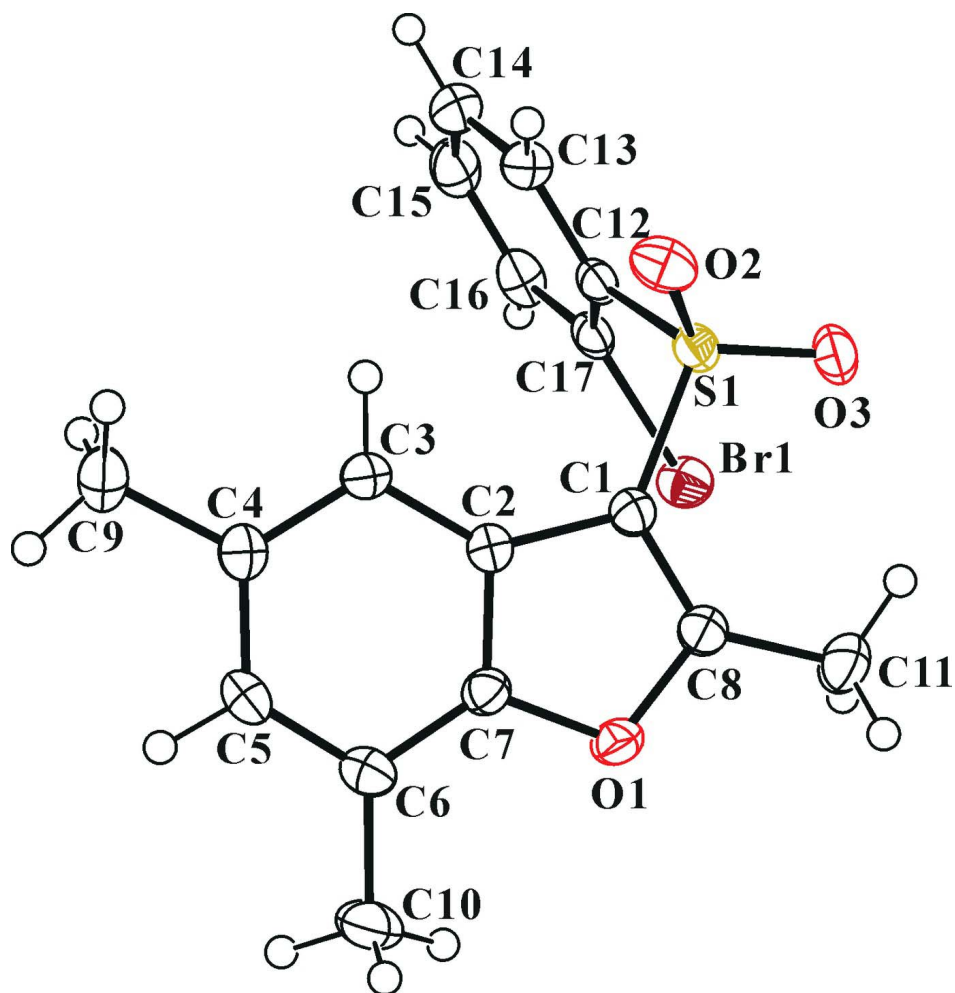
In the title molecule (Fig. 1), the benzofuran unit is essentially planar, with a mean deviation of 0.016 (2) Å from the least-squares plane defined by the nine constituent atoms. The 2-bromophenyl ring is essentially planar, with a mean deviation of 0.004 (2) Å from the least-squares plane defined by the six constituent atoms. The dihedral angle formed by the benzofuran ring and the 2-bromophenyl ring is 82.93 (6)°. In the crystal structure (Fig. 2), molecules are linked *via* two different pairs of C—H... $\pi$  hydrogen bonds (Table 1, Cg1 is the centroid of the C2–C7 benzene ring) and  $\pi$ – $\pi$  interactions between the benzene and furan rings of neighbouring molecules, with a Cg1...Cg2<sup>iii</sup> distance of 3.881 (2) Å and an interplanar distance of 3.562 (2) Å resulting in a slippage of 1.541 (2) Å (Cg2 is the centroid of the C1/C2/C7/O1/C8 furan ring), into inversion-related dimers along the *b*-axis direction. These dimers are further linked by halogen-bondings (Politzer *et al.* 2007) between the bromine and the O atom of the O=S=O unit [Br1...O3<sup>ii</sup> = 3.185 (2) Å, C17—Br1...O3<sup>ii</sup> = 164.49 (7)°, symmetry code: (ii) - *x* + 1/2, *y* - 1/2, - *z* + 3/2].

### S2. Experimental

The starting material 3-(2-bromophenylsulfonyl)-2,5,7-trimethyl-1-benzofuran was prepared by a literature method (Choi *et al.*, 1999). 3-Chloroperoxybenzoic acid (77%, 403 mg, 1.8 mmol) was added in small portions to a stirred solution of 3-(2-bromophenylsulfonyl)-2,5,7-trimethyl-1-benzofuran (278 mg, 0.8 mmol) in dichloromethane (30 ml) at 273 K. After being stirred at room temperature for 8h, the mixture was washed with saturated sodium bicarbonate solution (2 X 10 ml) and the organic layer was separated, dried over magnesium sulfate, filtered and concentrated at reduced pressure. The residue was purified by column chromatography (hexane-ethyl acetate, 4:1 *v/v*) to afford the title compound as a colorless solid [yield 72% (218 mg); m.p. 453–454 K; *R*<sub>f</sub> = 0.51 (hexane-ethyl acetate, 4:1 *v/v*)]. Single crystals suitable for X-ray diffraction were prepared by slow evaporation of a solution of the title compound (21 mg) in acetone (15 ml) at room temperature.

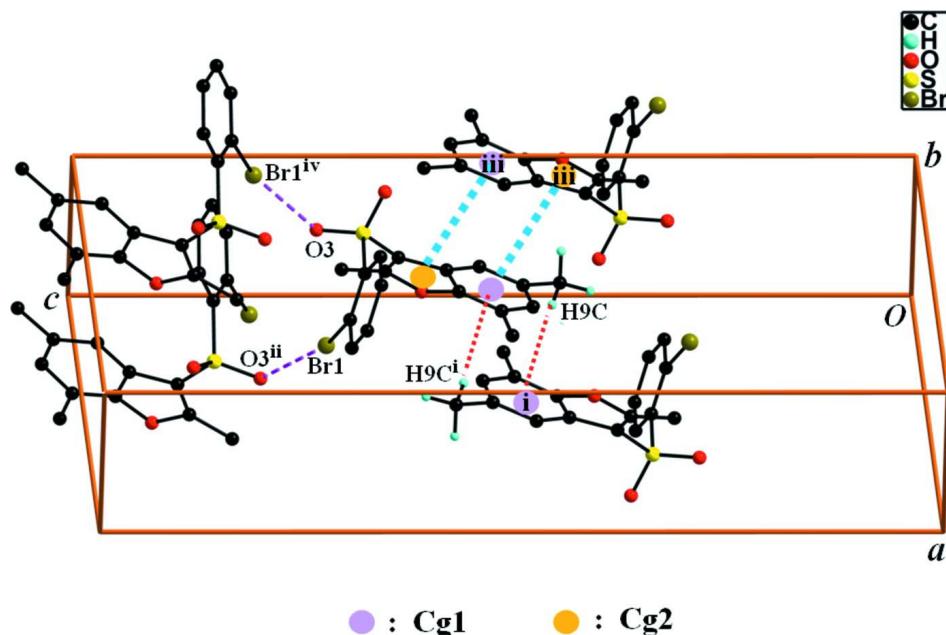
### S3. Refinement

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.95 Å for aryl, and 0.98 Å for methyl H atoms, respectively. *U*<sub>iso</sub> (H) = 1.2*U*<sub>eq</sub> (C) for aryl and 1.5*U*<sub>eq</sub> (C) for methyl H atoms. The positions of methyl hydrogens were optimized using the SHELXL-97's command AFIX 137 (Sheldrick, 2008).



**Figure 1**

The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are presented as small spheres of arbitrary radius.

**Figure 2**

A view of the C—H... $\pi$ ,  $\pi$ - $\pi$  and Br...O interactions (dotted lines) in the crystal structure of the title compound. H atoms non-participating in hydrogen-bonding were omitted for clarity. [Symmetry codes: (i)  $-x + 1, -y + 1, -z + 1$ ; (ii)  $-x + 1/2, y - 1/2, -z + 3/2$ ; (iii)  $-x, -y + 1, -z + 1$ ; (iv)  $-x + 1/2, y + 1/2, -z + 3/2$ .]

### 3-(2-Bromophenylsulfonyl)-2,5,7-trimethyl-1-benzofuran

#### Crystal data

$C_{17}H_{15}BrO_3S$

$M_r = 379.26$

Monoclinic,  $P2_1/n$

Hall symbol:  $-P\ 2_1n$

$a = 7.8969$  (2) Å

$b = 8.1489$  (2) Å

$c = 24.3146$  (6) Å

$\beta = 96.210$  (1)°

$V = 1555.49$  (7) Å<sup>3</sup>

$Z = 4$

$F(000) = 768$

$D_x = 1.619$  Mg m<sup>-3</sup>

Melting point = 454–453 K

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 7387 reflections

$\theta = 2.6$ – $26.1$ °

$\mu = 2.79$  mm<sup>-1</sup>

$T = 173$  K

Block, colourless

$0.31 \times 0.27 \times 0.13$  mm

#### Data collection

Bruker SMART APEXII CCD  
diffractometer

Radiation source: rotating anode

Graphite multilayer monochromator

Detector resolution: 10.0 pixels mm<sup>-1</sup>

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2009)

$T_{\min} = 0.479$ ,  $T_{\max} = 0.713$

27395 measured reflections

3867 independent reflections

3130 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.042$

$\theta_{\max} = 28.3$ °,  $\theta_{\min} = 1.7$ °

$h = -10 \rightarrow 10$

$k = -10 \rightarrow 10$

$l = -31 \rightarrow 32$

*Refinement*Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.031$  $wR(F^2) = 0.080$  $S = 1.03$ 

3867 reflections

202 parameters

0 restraints

Primary atom site location: structure-invariant  
direct methodsSecondary atom site location: difference Fourier  
map

Hydrogen site location: difference Fourier map

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0401P)^2 + 0.8758P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\max} = 0.001$  $\Delta\rho_{\max} = 0.51 \text{ e } \text{\AA}^{-3}$  $\Delta\rho_{\min} = -0.34 \text{ e } \text{\AA}^{-3}$ *Special details***Experimental.**  $^1\text{H}$  NMR ( $\delta$  p.p.m.,  $\text{CDCl}_3$ , 400 Hz): 8.49 (d,  $J = 6.12$  Hz, 1H), 7.65 (d,  $J = 6.84$  Hz, 1H), 7.53-7.58 (m, 1H), 7.38-7.43 (m, 1H), 7.06 (s, 1H), 6.88 (s, 1H), 2.84 (s, 3H), 2.43 (s, 3H), 2.31 (s, 3H).**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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.46256 (3)	0.42412 (3)	0.713662 (9)	0.03093 (9)
S1	0.12638 (7)	0.65915 (7)	0.65837 (2)	0.02299 (13)
O1	0.1202 (2)	0.22941 (18)	0.58642 (6)	0.0280 (4)
O2	0.0262 (2)	0.7852 (2)	0.62933 (7)	0.0320 (4)
O3	0.0830 (2)	0.6094 (2)	0.71169 (7)	0.0311 (4)
C1	0.1294 (3)	0.4896 (3)	0.61574 (9)	0.0222 (4)
C2	0.1822 (3)	0.4890 (3)	0.56071 (8)	0.0208 (4)
C3	0.2360 (3)	0.6058 (3)	0.52431 (9)	0.0241 (4)
H3	0.2402	0.7190	0.5337	0.029*
C4	0.2832 (3)	0.5521 (3)	0.47408 (9)	0.0257 (5)
C5	0.2767 (3)	0.3855 (3)	0.46099 (9)	0.0273 (5)
H5	0.3106	0.3521	0.4264	0.033*
C6	0.2235 (3)	0.2660 (3)	0.49579 (9)	0.0270 (5)
C7	0.1761 (3)	0.3251 (3)	0.54484 (9)	0.0229 (4)
C8	0.0946 (3)	0.3321 (3)	0.62932 (9)	0.0258 (5)
C9	0.3440 (3)	0.6725 (3)	0.43345 (10)	0.0350 (6)
H9A	0.2662	0.7664	0.4294	0.053*
H9B	0.3467	0.6188	0.3975	0.053*
H9C	0.4587	0.7105	0.4470	0.053*
C10	0.2218 (4)	0.0869 (3)	0.48191 (12)	0.0412 (6)
H10A	0.2464	0.0228	0.5159	0.062*
H10B	0.3084	0.0642	0.4570	0.062*
H10C	0.1093	0.0566	0.4638	0.062*

C11	0.0392 (3)	0.2511 (3)	0.67846 (10)	0.0378 (6)
H11A	0.1317	0.1821	0.6958	0.057*
H11B	-0.0608	0.1827	0.6674	0.057*
H11C	0.0099	0.3344	0.7049	0.057*
C12	0.3401 (3)	0.7318 (3)	0.66497 (8)	0.0220 (4)
C13	0.3630 (3)	0.8918 (3)	0.64809 (10)	0.0286 (5)
H13	0.2678	0.9543	0.6327	0.034*
C14	0.5241 (3)	0.9611 (3)	0.65352 (11)	0.0365 (6)
H14	0.5390	1.0714	0.6423	0.044*
C15	0.6626 (3)	0.8704 (3)	0.67508 (11)	0.0363 (6)
H15	0.7730	0.9181	0.6785	0.044*
C16	0.6417 (3)	0.7101 (3)	0.69174 (10)	0.0315 (5)
H16	0.7377	0.6476	0.7063	0.038*
C17	0.4809 (3)	0.6409 (3)	0.68725 (9)	0.0238 (4)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Br1	0.03549 (14)	0.02720 (13)	0.02903 (14)	0.00525 (10)	-0.00148 (9)	0.00300 (9)
S1	0.0223 (3)	0.0245 (3)	0.0227 (3)	0.0008 (2)	0.0050 (2)	-0.0029 (2)
O1	0.0390 (9)	0.0201 (7)	0.0247 (8)	-0.0047 (7)	0.0030 (7)	0.0020 (6)
O2	0.0277 (8)	0.0306 (9)	0.0366 (9)	0.0082 (7)	-0.0009 (7)	-0.0044 (7)
O3	0.0319 (8)	0.0388 (10)	0.0243 (8)	-0.0031 (7)	0.0113 (7)	-0.0042 (7)
C1	0.0231 (10)	0.0228 (10)	0.0209 (11)	-0.0007 (8)	0.0030 (8)	-0.0005 (8)
C2	0.0197 (10)	0.0225 (10)	0.0201 (10)	0.0011 (8)	0.0018 (8)	0.0005 (8)
C3	0.0275 (11)	0.0204 (10)	0.0244 (11)	-0.0008 (8)	0.0033 (9)	-0.0006 (8)
C4	0.0248 (11)	0.0295 (11)	0.0229 (11)	0.0006 (9)	0.0031 (9)	0.0018 (9)
C5	0.0304 (11)	0.0307 (12)	0.0214 (11)	0.0033 (9)	0.0052 (9)	-0.0048 (9)
C6	0.0299 (11)	0.0255 (11)	0.0248 (12)	0.0019 (9)	-0.0001 (9)	-0.0043 (9)
C7	0.0258 (11)	0.0208 (10)	0.0217 (11)	-0.0016 (8)	0.0012 (8)	0.0016 (8)
C8	0.0282 (11)	0.0258 (11)	0.0236 (11)	-0.0030 (9)	0.0031 (9)	-0.0012 (9)
C9	0.0391 (14)	0.0392 (14)	0.0283 (13)	-0.0014 (11)	0.0106 (11)	0.0039 (11)
C10	0.0618 (18)	0.0252 (12)	0.0368 (15)	0.0020 (12)	0.0065 (13)	-0.0082 (11)
C11	0.0508 (16)	0.0351 (13)	0.0288 (13)	-0.0102 (12)	0.0098 (11)	0.0050 (11)
C12	0.0242 (10)	0.0244 (11)	0.0180 (10)	-0.0011 (8)	0.0055 (8)	-0.0046 (8)
C13	0.0346 (12)	0.0241 (11)	0.0278 (12)	0.0005 (9)	0.0057 (10)	-0.0006 (9)
C14	0.0477 (15)	0.0286 (12)	0.0349 (14)	-0.0092 (11)	0.0124 (12)	-0.0037 (10)
C15	0.0308 (12)	0.0455 (15)	0.0339 (14)	-0.0116 (11)	0.0085 (11)	-0.0094 (12)
C16	0.0256 (11)	0.0428 (14)	0.0261 (12)	0.0003 (10)	0.0034 (9)	-0.0053 (10)
C17	0.0293 (11)	0.0262 (11)	0.0163 (10)	0.0023 (9)	0.0044 (8)	-0.0027 (8)

*Geometric parameters (Å, °)*

Br1—C17	1.890 (2)	C8—C11	1.472 (3)
Br1—O3 <sup>i</sup>	22.6093 (17)	C9—H9A	0.9800
S1—O3	1.4345 (16)	C9—H9B	0.9800
S1—O2	1.4348 (17)	C9—H9C	0.9800
S1—C1	1.729 (2)	C10—H10A	0.9800

S1—C12	1.779 (2)	C10—H10B	0.9800
O1—C8	1.369 (3)	C10—H10C	0.9800
O1—C7	1.386 (3)	C11—H11A	0.9800
C1—C8	1.361 (3)	C11—H11B	0.9800
C1—C2	1.444 (3)	C11—H11C	0.9800
C2—C7	1.390 (3)	C12—C13	1.385 (3)
C2—C3	1.397 (3)	C12—C17	1.396 (3)
C3—C4	1.386 (3)	C13—C14	1.385 (4)
C3—H3	0.9500	C13—H13	0.9500
C4—C5	1.395 (3)	C14—C15	1.376 (4)
C4—C9	1.507 (3)	C14—H14	0.9500
C5—C6	1.385 (3)	C15—C16	1.383 (4)
C5—H5	0.9500	C15—H15	0.9500
C6—C7	1.375 (3)	C16—C17	1.383 (3)
C6—C10	1.497 (3)	C16—H16	0.9500
C17—Br1—O3 <sup>‡</sup>	76.20 (6)	H9A—C9—H9B	109.5
O3—S1—O2	118.32 (10)	C4—C9—H9C	109.5
O3—S1—C1	109.64 (10)	H9A—C9—H9C	109.5
O2—S1—C1	108.65 (10)	H9B—C9—H9C	109.5
O3—S1—C12	109.22 (10)	C6—C10—H10A	109.5
O2—S1—C12	105.85 (10)	C6—C10—H10B	109.5
C1—S1—C12	104.19 (10)	H10A—C10—H10B	109.5
C8—O1—C7	107.27 (16)	C6—C10—H10C	109.5
C8—C1—C2	107.93 (19)	H10A—C10—H10C	109.5
C8—C1—S1	126.30 (17)	H10B—C10—H10C	109.5
C2—C1—S1	125.62 (16)	C8—C11—H11A	109.5
C7—C2—C3	118.87 (19)	C8—C11—H11B	109.5
C7—C2—C1	104.80 (18)	H11A—C11—H11B	109.5
C3—C2—C1	136.3 (2)	C8—C11—H11C	109.5
C4—C3—C2	118.2 (2)	H11A—C11—H11C	109.5
C4—C3—H3	120.9	H11B—C11—H11C	109.5
C2—C3—H3	120.9	C13—C12—C17	119.4 (2)
C3—C4—C5	120.1 (2)	C13—C12—S1	116.07 (17)
C3—C4—C9	120.5 (2)	C17—C12—S1	124.50 (17)
C5—C4—C9	119.4 (2)	C12—C13—C14	120.3 (2)
C6—C5—C4	123.5 (2)	C12—C13—H13	119.9
C6—C5—H5	118.3	C14—C13—H13	119.9
C4—C5—H5	118.3	C15—C14—C13	120.1 (2)
C7—C6—C5	114.4 (2)	C15—C14—H14	120.0
C7—C6—C10	122.7 (2)	C13—C14—H14	120.0
C5—C6—C10	122.9 (2)	C14—C15—C16	120.3 (2)
C6—C7—O1	125.00 (19)	C14—C15—H15	119.9
C6—C7—C2	124.9 (2)	C16—C15—H15	119.9
O1—C7—C2	110.03 (18)	C17—C16—C15	120.0 (2)
C1—C8—O1	109.95 (18)	C17—C16—H16	120.0
C1—C8—C11	134.9 (2)	C15—C16—H16	120.0
O1—C8—C11	115.2 (2)	C16—C17—C12	120.0 (2)

C4—C9—H9A	109.5	C16—C17—Br1	117.25 (18)
C4—C9—H9B	109.5	C12—C17—Br1	122.73 (17)
O3—S1—C1—C8	0.8 (2)	C1—C2—C7—O1	1.1 (2)
O2—S1—C1—C8	-129.9 (2)	C2—C1—C8—O1	-0.4 (2)
C12—S1—C1—C8	117.6 (2)	S1—C1—C8—O1	-176.16 (16)
O3—S1—C1—C2	-174.23 (18)	C2—C1—C8—C11	178.8 (3)
O2—S1—C1—C2	55.1 (2)	S1—C1—C8—C11	3.0 (4)
C12—S1—C1—C2	-57.4 (2)	C7—O1—C8—C1	1.1 (2)
C8—C1—C2—C7	-0.4 (2)	C7—O1—C8—C11	-178.3 (2)
S1—C1—C2—C7	175.34 (16)	O3—S1—C12—C13	-121.32 (17)
C8—C1—C2—C3	-178.9 (2)	O2—S1—C12—C13	7.10 (19)
S1—C1—C2—C3	-3.1 (4)	C1—S1—C12—C13	121.60 (18)
C7—C2—C3—C4	-0.8 (3)	O3—S1—C12—C17	56.5 (2)
C1—C2—C3—C4	177.4 (2)	O2—S1—C12—C17	-175.07 (17)
C2—C3—C4—C5	-0.1 (3)	C1—S1—C12—C17	-60.6 (2)
C2—C3—C4—C9	-179.4 (2)	C17—C12—C13—C14	-0.3 (3)
C3—C4—C5—C6	0.4 (4)	S1—C12—C13—C14	177.65 (18)
C9—C4—C5—C6	179.7 (2)	C12—C13—C14—C15	0.8 (4)
C4—C5—C6—C7	0.3 (3)	C13—C14—C15—C16	-0.4 (4)
C4—C5—C6—C10	-178.2 (2)	C14—C15—C16—C17	-0.6 (4)
C5—C6—C7—O1	-179.3 (2)	C15—C16—C17—C12	1.2 (3)
C10—C6—C7—O1	-0.8 (4)	C15—C16—C17—Br1	-177.56 (18)
C5—C6—C7—C2	-1.4 (3)	C13—C12—C17—C16	-0.7 (3)
C10—C6—C7—C2	177.2 (2)	S1—C12—C17—C16	-178.47 (17)
C8—O1—C7—C6	176.8 (2)	C13—C12—C17—Br1	177.95 (16)
C8—O1—C7—C2	-1.4 (2)	S1—C12—C17—Br1	0.2 (3)
C3—C2—C7—C6	1.7 (3)	O3 <sup>i</sup> —Br1—C17—C16	-99.99 (17)
C1—C2—C7—C6	-177.1 (2)	O3 <sup>i</sup> —Br1—C17—C12	81.32 (17)
C3—C2—C7—O1	179.89 (18)		

Symmetry code: (i)  $-x+1/2, y-1/2, -z+1/2$ .

#### Hydrogen-bond geometry ( $\text{\AA}, ^\circ$ )

Cg1 is the centroid of the C2—C7 benzene ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C9—H9C <sup>ii</sup> —Cg1 <sup>ii</sup>	0.98	2.84	3.608 (2)	136

Symmetry code: (ii)  $-x+1, -y+1, -z+1$ .