

$\alpha = 76.763(2)^\circ$
 $\beta = 84.145(2)^\circ$
 $\gamma = 73.241(2)^\circ$
 $V = 754.73(4)\text{ \AA}^3$
 $Z = 2$

Mo $K\alpha$ radiation
 $\mu = 0.39\text{ mm}^{-1}$
 $T = 173\text{ K}$
 $0.28 \times 0.25 \times 0.21\text{ mm}$

3-(3-Chlorophenylsulfinyl)-2,4,6-trimethyl-1-benzofuran

Hong Dae Choi,^a Pil Ja Seo^a and Uk Lee^{b*}

^aDepartment of Chemistry, Dongeui University, San 24 Kaya-dong Busanjin-gu, Busan 614-714, Republic of Korea, and ^bDepartment of Chemistry, Pukyong National University, 599-1 Daeyeon 3-dong, Nam-gu, Busan 608-737, Republic of Korea
Correspondence e-mail: uklee@pknu.ac.kr

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Key indicators: single-crystal X-ray study; $T = 173\text{ K}$; mean $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$; R factor = 0.037; wR factor = 0.105; data-to-parameter ratio = 19.2.

In the title compound, $C_{17}H_{15}ClO_2S$, the 3-chlorophenyl ring makes a dihedral angle of $71.46(4)^\circ$ with the mean plane of the benzofuran fragment. In the crystal, molecules are linked by weak C—H···O hydrogen bonds and a slipped π – π interaction between the 3-chlorophenyl rings of adjacent molecules [centroid–centroid distance = $3.630(2)\text{ \AA}$, interplanar distance = $3.375(2)\text{ \AA}$ and slippage = $1.337(2)\text{ \AA}$].

Related literature

For the pharmacological activity of benzofuran compounds, see: Aslam *et al.* (2009); Galal *et al.* (2009); Khan *et al.* (2005). For natural products with benzofuran rings, see: Akgul & Anil (2003); Soekamto *et al.* (2003). For the crystal structures of related compounds, see: Choi *et al.* (2010); Seo *et al.* (2011).

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
 $R_{\text{int}} = 0.030$
 $T_{\min} = 0.675$, $T_{\max} = 0.746$

14017 measured reflections
3704 independent reflections
3182 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.105$
 $S = 1.05$
3704 reflections

193 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.33\text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.42\text{ e \AA}^{-3}$

Table 1
Hydrogen-bond geometry (\AA , $^\circ$).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
C11—H11B···O2 ⁱ	0.98	2.30	3.249 (2)	163

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

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* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2502).

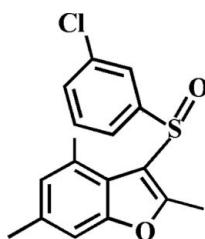
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Experimental

Crystal data

$C_{17}H_{15}ClO_2S$
 $M_r = 318.80$
Triclinic, $P\bar{1}$
 $a = 6.7900(2)\text{ \AA}$
 $b = 8.1288(3)\text{ \AA}$
 $c = 14.6813(5)\text{ \AA}$



supplementary materials

Acta Cryst. (2012), E68, o374 [doi:10.1107/S160053681200027X]

3-(3-Chlorophenylsulfinyl)-2,4,6-trimethyl-1-benzofuran

H. D. Choi, P. J. Seo and U. Lee

Comment

Many compounds involving benzofuran skeleton have drawn much attention owing to their valuable biological properties such as antibacterial and antifungal, antitumor and antiviral, and antimicrobial activities (Aslam *et al.*, 2009, Galal *et al.*, 2009, Khan *et al.*, 2005). These benzofuran derivatives occur in a wide range of natural products (Akgul & Anil, 2003; Soekamto *et al.*, 2003). As a part of our ongoing study of 2, 4, 6-trimethyl-1-benzofuran derivatives containing either 3-(4-chlorophenylsulfinyl) (Choi *et al.*, 2010) or 3-(3-fluorophenylsulfinyl) (Seo *et al.*, 2011) substituents, we report herein the crystal structure of the title compound.

In the title molecule (Fig. 1), the benzofuran unit is essentially planar, with a mean deviation of 0.005 (1) Å from the least-squares plane defined by the nine constituent atoms. The dihedral angle between the 3-chlorophenyl ring and the mean plane of the benzofuran fragment is 71.46 (4)°. The crystal packing (Fig. 2) is stabilized by weak intermolecular C—H···O hydrogen bonds (Table 1). The crystal packing (Fig. 2) is further stabilized by a weak slipped π–π interaction between the 3-chlorophenyl rings of adjacent molecules, with a Cg···Cgⁱⁱ distance of 3.630 (2) Å and an interplanar distance of 3.375 (2) Å resulting in a slippage of 1.337 (2) Å (Cg is the centroid of the C12-C17 3-chlorophenyl ring).

Experimental

77% 3-Chloroperoxybenzoic acid (269 mg, 1.3 mmol) was added in small portions to a stirred solution of 3-(3-chlorophenylsulfinyl)-2,4,6-trimethyl 1-benzofuran (333 mg, 1.1 mmol) in dichloromethane (40 mL) at 273 K. After being stirred at room temperature for 5 h, the mixture was washed with saturated sodium bicarbonate solution 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, 2:1 v/v) to afford the title compound as a colorless solid [yield 73%, m.p. 402–403 K; R_f = 0.53 (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 in acetone at room temperature.

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. $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for aryl and $1.5U_{\text{eq}}(\text{C})$ for methyl H atoms.

supplementary materials

Figures

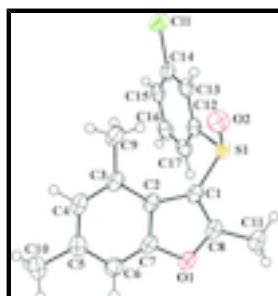


Fig. 1. The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are presented as small spheres of arbitrary radius.

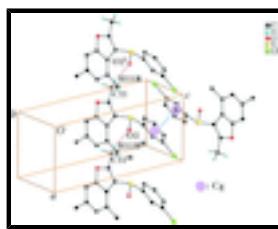


Fig. 2. A view of the C—H···O and π ··· π interactions (dotted lines) in the crystal structure of the title compound. H atoms not participating in hydrogen-bonding were omitted for clarity. [Symmetry codes: (i) $x - 1, y, z$; (ii) $-x + 1, -y + 1, -z + 2$; (iii) $x + 1, y, z$.]

3-(3-Chlorophenylsulfinyl)-2,4,6-trimethyl-1-benzofuran

Crystal data

C ₁₇ H ₁₅ ClO ₂ S	Z = 2
M _r = 318.80	F(000) = 332
Triclinic, PT	D _x = 1.403 Mg m ⁻³
Hall symbol: -P 1	Mo K α radiation, λ = 0.71073 Å
a = 6.7900 (2) Å	Cell parameters from 6373 reflections
b = 8.1288 (3) Å	θ = 2.7–28.1°
c = 14.6813 (5) Å	μ = 0.39 mm ⁻¹
α = 76.763 (2)°	T = 173 K
β = 84.145 (2)°	Block, colourless
γ = 73.241 (2)°	0.28 × 0.25 × 0.21 mm
V = 754.73 (4) Å ³	

Data collection

Bruker SMART APEXII CCD diffractometer	3704 independent reflections
Radiation source: rotating anode graphite multilayer	3182 reflections with $I > 2\sigma(I)$
Detector resolution: 10.0 pixels mm ⁻¹	$R_{\text{int}} = 0.030$
φ and ω scans	$\theta_{\text{max}} = 28.3^\circ$, $\theta_{\text{min}} = 1.4^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2009)	$h = -9 \rightarrow 9$
$T_{\text{min}} = 0.675$, $T_{\text{max}} = 0.746$	$k = -10 \rightarrow 10$
14017 measured reflections	$l = -19 \rightarrow 19$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.037$	Hydrogen site location: difference Fourier map
$wR(F^2) = 0.105$	H-atom parameters constrained
$S = 1.05$	$w = 1/[\sigma^2(F_o^2) + (0.0546P)^2 + 0.219P]$ where $P = (F_o^2 + 2F_c^2)/3$
3704 reflections	$(\Delta/\sigma)_{\max} = 0.001$
193 parameters	$\Delta\rho_{\max} = 0.33 \text{ e \AA}^{-3}$
0 restraints	$\Delta\rho_{\min} = -0.42 \text{ e \AA}^{-3}$

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 $F^2 > 2\text{sigma}(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	0.98398 (6)	0.23182 (6)	0.99982 (3)	0.04624 (14)
S1	0.46056 (6)	0.83926 (5)	0.83535 (3)	0.03407 (12)
O1	0.14598 (16)	0.96772 (15)	0.61039 (8)	0.0363 (3)
O2	0.65568 (19)	0.88857 (16)	0.83626 (9)	0.0443 (3)
C1	0.3829 (2)	0.8720 (2)	0.72075 (11)	0.0312 (3)
C2	0.4775 (2)	0.80409 (19)	0.63819 (10)	0.0300 (3)
C3	0.6724 (2)	0.7063 (2)	0.61075 (11)	0.0336 (3)
C4	0.6909 (2)	0.6719 (2)	0.52105 (12)	0.0368 (3)
H4	0.8208	0.6054	0.5009	0.044*
C5	0.5309 (3)	0.7288 (2)	0.45904 (11)	0.0367 (3)
C6	0.3406 (3)	0.8309 (2)	0.48513 (11)	0.0375 (3)
H6	0.2289	0.8745	0.4442	0.045*
C7	0.3229 (2)	0.8653 (2)	0.57378 (11)	0.0325 (3)
C8	0.1876 (2)	0.9692 (2)	0.69925 (11)	0.0336 (3)
C9	0.8536 (3)	0.6437 (3)	0.67277 (13)	0.0448 (4)
H9A	0.8515	0.5309	0.7141	0.067*
H9B	0.8462	0.7303	0.7106	0.067*
H9C	0.9813	0.6291	0.6340	0.067*
C10	0.5634 (3)	0.6788 (3)	0.36442 (12)	0.0464 (4)

supplementary materials

H10A	0.5396	0.5633	0.3706	0.070*
H10B	0.7047	0.6741	0.3408	0.070*
H10C	0.4667	0.7665	0.3205	0.070*
C11	0.0176 (3)	1.0752 (2)	0.75130 (13)	0.0432 (4)
H11A	0.0667	1.0788	0.8111	0.065*
H11B	-0.0972	1.0217	0.7630	0.065*
H11C	-0.0288	1.1950	0.7141	0.065*
C12	0.5290 (2)	0.6027 (2)	0.86348 (10)	0.0302 (3)
C13	0.7090 (2)	0.5182 (2)	0.91058 (10)	0.0317 (3)
H13	0.7954	0.5830	0.9234	0.038*
C14	0.7601 (2)	0.3376 (2)	0.93850 (11)	0.0326 (3)
C15	0.6376 (2)	0.2399 (2)	0.92032 (11)	0.0339 (3)
H15	0.6762	0.1155	0.9394	0.041*
C16	0.4574 (3)	0.3280 (2)	0.87360 (11)	0.0355 (3)
H16	0.3716	0.2629	0.8606	0.043*
C17	0.4002 (2)	0.5095 (2)	0.84550 (11)	0.0339 (3)
H17	0.2753	0.5690	0.8145	0.041*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0373 (2)	0.0353 (2)	0.0654 (3)	-0.00594 (17)	-0.00790 (18)	-0.01169 (19)
S1	0.0379 (2)	0.0264 (2)	0.0417 (2)	-0.00941 (16)	0.00082 (15)	-0.01471 (16)
O1	0.0268 (5)	0.0343 (6)	0.0432 (6)	-0.0021 (4)	0.0024 (4)	-0.0087 (5)
O2	0.0469 (7)	0.0333 (6)	0.0612 (8)	-0.0190 (5)	-0.0072 (6)	-0.0144 (6)
C1	0.0296 (7)	0.0248 (7)	0.0394 (8)	-0.0070 (6)	0.0034 (6)	-0.0094 (6)
C2	0.0298 (7)	0.0223 (7)	0.0373 (7)	-0.0073 (6)	0.0040 (6)	-0.0072 (6)
C3	0.0305 (7)	0.0252 (7)	0.0434 (8)	-0.0060 (6)	0.0043 (6)	-0.0085 (6)
C4	0.0348 (8)	0.0281 (8)	0.0443 (8)	-0.0054 (6)	0.0103 (6)	-0.0105 (6)
C5	0.0432 (9)	0.0302 (8)	0.0367 (8)	-0.0127 (7)	0.0082 (6)	-0.0083 (6)
C6	0.0379 (8)	0.0339 (9)	0.0378 (8)	-0.0083 (7)	-0.0003 (6)	-0.0043 (6)
C7	0.0286 (7)	0.0254 (7)	0.0401 (8)	-0.0048 (6)	0.0045 (6)	-0.0061 (6)
C8	0.0307 (7)	0.0277 (8)	0.0417 (8)	-0.0075 (6)	0.0055 (6)	-0.0094 (6)
C9	0.0308 (8)	0.0460 (10)	0.0539 (10)	0.0006 (7)	0.0003 (7)	-0.0179 (8)
C10	0.0565 (11)	0.0459 (11)	0.0392 (9)	-0.0175 (9)	0.0098 (8)	-0.0144 (8)
C11	0.0331 (8)	0.0382 (9)	0.0551 (10)	-0.0038 (7)	0.0090 (7)	-0.0161 (8)
C12	0.0358 (7)	0.0257 (7)	0.0325 (7)	-0.0109 (6)	0.0039 (6)	-0.0124 (6)
C13	0.0338 (7)	0.0301 (8)	0.0365 (8)	-0.0126 (6)	0.0022 (6)	-0.0139 (6)
C14	0.0315 (7)	0.0315 (8)	0.0360 (7)	-0.0069 (6)	0.0035 (6)	-0.0137 (6)
C15	0.0429 (8)	0.0262 (8)	0.0358 (7)	-0.0111 (6)	0.0057 (6)	-0.0139 (6)
C16	0.0432 (8)	0.0341 (8)	0.0381 (8)	-0.0196 (7)	0.0034 (6)	-0.0161 (6)
C17	0.0367 (8)	0.0353 (8)	0.0348 (7)	-0.0139 (7)	-0.0002 (6)	-0.0130 (6)

Geometric parameters (\AA , $^\circ$)

Cl1—C14	1.7412 (16)	C9—H9A	0.9800
S1—O2	1.4928 (12)	C9—H9B	0.9800
S1—C1	1.7534 (16)	C9—H9C	0.9800
S1—C12	1.8009 (15)	C10—H10A	0.9800

O1—C8	1.3661 (19)	C10—H10B	0.9800
O1—C7	1.3863 (18)	C10—H10C	0.9800
C1—C8	1.360 (2)	C11—H11A	0.9800
C1—C2	1.459 (2)	C11—H11B	0.9800
C2—C7	1.389 (2)	C11—H11C	0.9800
C2—C3	1.406 (2)	C12—C13	1.384 (2)
C3—C4	1.394 (2)	C12—C17	1.389 (2)
C3—C9	1.502 (2)	C13—C14	1.380 (2)
C4—C5	1.393 (2)	C13—H13	0.9500
C4—H4	0.9500	C14—C15	1.384 (2)
C5—C6	1.390 (2)	C15—C16	1.386 (2)
C5—C10	1.513 (2)	C15—H15	0.9500
C6—C7	1.379 (2)	C16—C17	1.386 (2)
C6—H6	0.9500	C16—H16	0.9500
C8—C11	1.486 (2)	C17—H17	0.9500
O2—S1—C1	111.41 (7)	H9A—C9—H9C	109.5
O2—S1—C12	106.01 (7)	H9B—C9—H9C	109.5
C1—S1—C12	98.39 (7)	C5—C10—H10A	109.5
C8—O1—C7	106.59 (12)	C5—C10—H10B	109.5
C8—C1—C2	107.12 (14)	H10A—C10—H10B	109.5
C8—C1—S1	118.56 (12)	C5—C10—H10C	109.5
C2—C1—S1	134.08 (12)	H10A—C10—H10C	109.5
C7—C2—C3	118.49 (14)	H10B—C10—H10C	109.5
C7—C2—C1	104.44 (13)	C8—C11—H11A	109.5
C3—C2—C1	137.02 (14)	C8—C11—H11B	109.5
C4—C3—C2	116.22 (15)	H11A—C11—H11B	109.5
C4—C3—C9	121.02 (14)	C8—C11—H11C	109.5
C2—C3—C9	122.75 (14)	H11A—C11—H11C	109.5
C5—C4—C3	124.16 (15)	H11B—C11—H11C	109.5
C5—C4—H4	117.9	C13—C12—C17	121.25 (14)
C3—C4—H4	117.9	C13—C12—S1	116.72 (11)
C6—C5—C4	119.45 (15)	C17—C12—S1	121.85 (12)
C6—C5—C10	120.21 (16)	C14—C13—C12	118.42 (13)
C4—C5—C10	120.34 (15)	C14—C13—H13	120.8
C7—C6—C5	116.27 (15)	C12—C13—H13	120.8
C7—C6—H6	121.9	C13—C14—C15	121.98 (15)
C5—C6—H6	121.9	C13—C14—Cl1	118.34 (12)
C6—C7—O1	123.93 (14)	C15—C14—Cl1	119.67 (12)
C6—C7—C2	125.32 (14)	C14—C15—C16	118.42 (14)
O1—C7—C2	110.75 (13)	C14—C15—H15	120.8
C1—C8—O1	111.09 (13)	C16—C15—H15	120.8
C1—C8—C11	133.38 (16)	C17—C16—C15	121.11 (14)
O1—C8—C11	115.53 (14)	C17—C16—H16	119.4
C3—C9—H9A	109.5	C15—C16—H16	119.4
C3—C9—H9B	109.5	C16—C17—C12	118.80 (15)
H9A—C9—H9B	109.5	C16—C17—H17	120.6
C3—C9—H9C	109.5	C12—C17—H17	120.6
O2—S1—C1—C8	-127.62 (13)	C1—C2—C7—C6	-178.73 (15)

supplementary materials

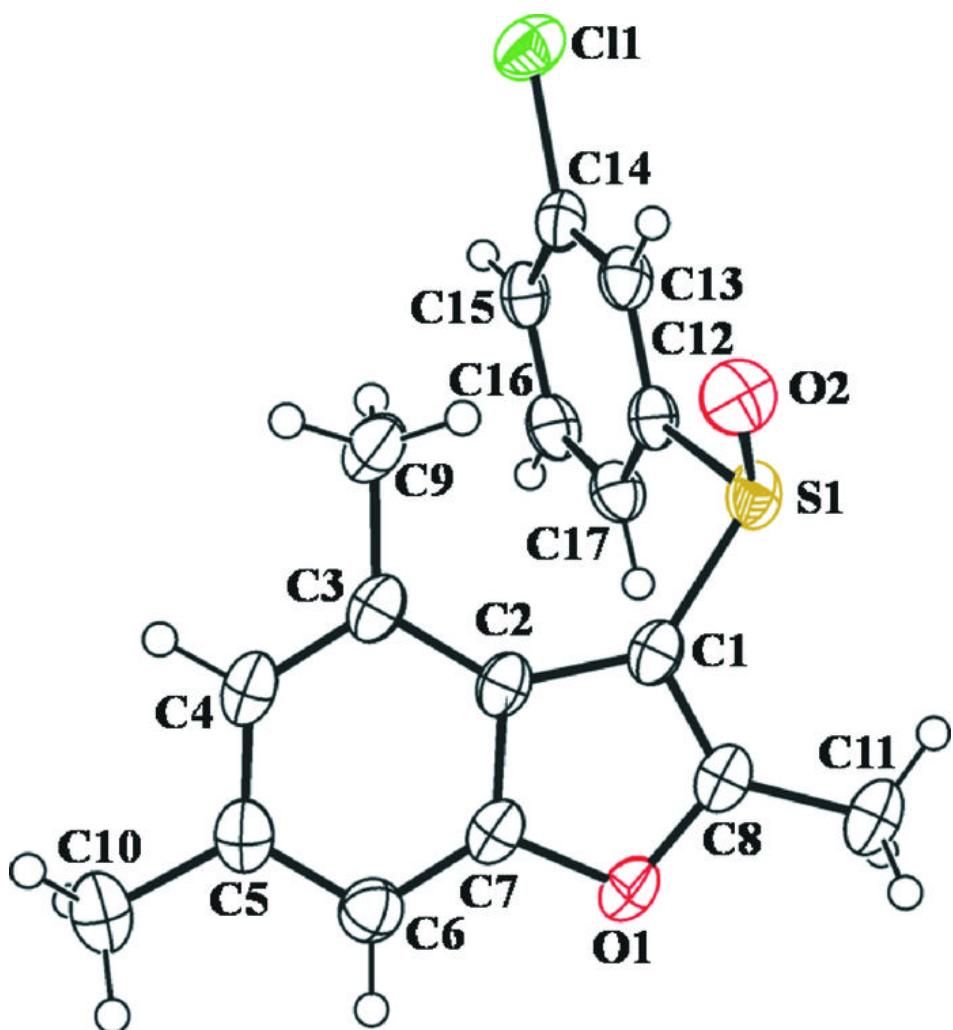
C12—S1—C1—C8	121.46 (13)	C3—C2—C7—O1	-176.29 (13)
O2—S1—C1—C2	58.83 (17)	C1—C2—C7—O1	1.51 (16)
C12—S1—C1—C2	-52.10 (16)	C2—C1—C8—O1	1.05 (17)
C8—C1—C2—C7	-1.54 (16)	S1—C1—C8—O1	-174.11 (10)
S1—C1—C2—C7	172.54 (13)	C2—C1—C8—C11	-177.87 (17)
C8—C1—C2—C3	175.63 (17)	S1—C1—C8—C11	7.0 (3)
S1—C1—C2—C3	-10.3 (3)	C7—O1—C8—C1	-0.11 (17)
C7—C2—C3—C4	-2.9 (2)	C7—O1—C8—C11	179.01 (13)
C1—C2—C3—C4	-179.79 (16)	O2—S1—C12—C13	22.00 (13)
C7—C2—C3—C9	176.05 (15)	C1—S1—C12—C13	137.22 (12)
C1—C2—C3—C9	-0.8 (3)	O2—S1—C12—C17	-162.87 (12)
C2—C3—C4—C5	0.4 (2)	C1—S1—C12—C17	-47.65 (13)
C9—C3—C4—C5	-178.61 (16)	C17—C12—C13—C14	0.9 (2)
C3—C4—C5—C6	1.9 (2)	S1—C12—C13—C14	176.04 (11)
C3—C4—C5—C10	-177.54 (15)	C12—C13—C14—C15	0.3 (2)
C4—C5—C6—C7	-1.5 (2)	C12—C13—C14—Cl1	-178.73 (11)
C10—C5—C6—C7	177.93 (14)	C13—C14—C15—C16	-0.8 (2)
C5—C6—C7—O1	178.59 (14)	Cl1—C14—C15—C16	178.26 (12)
C5—C6—C7—C2	-1.1 (2)	C14—C15—C16—C17	0.1 (2)
C8—O1—C7—C6	179.30 (15)	C15—C16—C17—C12	1.1 (2)
C8—O1—C7—C2	-0.93 (16)	C13—C12—C17—C16	-1.6 (2)
C3—C2—C7—C6	3.5 (2)	S1—C12—C17—C16	-176.51 (12)

Hydrogen-bond geometry (\AA , $^\circ$)

$D\text{—H}\cdots A$	$D\text{—H}$	$H\cdots A$	$D\cdots A$	$D\text{—H}\cdots A$
C11—H11B \cdots O2 ⁱ	0.98	2.30	3.249 (2)	163.

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

Fig. 1



supplementary materials

Fig. 2

