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5-Cyclopentyl-2-methyl-3-phenyl-sulfonyl-1-benzofuran

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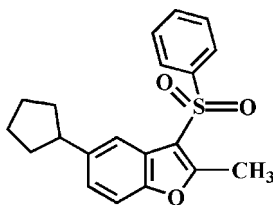
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 Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.052; wR factor = 0.130; data-to-parameter ratio = 16.6.

In the title compound, $\text{C}_{20}\text{H}_{20}\text{O}_3\text{S}$, the cyclopentyl ring adopts an envelope conformation. The phenyl ring makes a dihedral angle of $81.40(6)^\circ$ with the mean plane of the benzofuran fragment. In the crystal, molecules are linked by weak intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds and $\text{C}-\text{H}\cdots\pi$ interactions.

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 structural studies of related 5-alkyl-2-methyl-3-phenylsulfonyl-1-benzofuran derivatives, see: Choi *et al.* (2008a,b); Seo *et al.* (2011).



Experimental

Crystal data

 $\text{C}_{20}\text{H}_{20}\text{O}_3\text{S}$
 $M_r = 340.42$
 Monoclinic, $P2_1/c$
 $a = 6.2999(9)$ Å
 $b = 15.001(2)$ Å
 $c = 17.743(2)$ Å

 $\beta = 92.011(3)^\circ$
 $V = 1675.8(4)$ Å³
 $Z = 4$
 Mo $K\alpha$ radiation

 $\mu = 0.21$ mm⁻¹
 $T = 173$ K
 $0.27 \times 0.10 \times 0.08$ mm

Data collection

 Bruker SMART APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2009)
 $T_{\min} = 0.946$, $T_{\max} = 0.983$

 15497 measured reflections
 3616 independent reflections
 2869 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.065$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.052$
 $wR(F^2) = 0.130$
 $S = 1.04$
 3616 reflections

 218 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.44$ e Å⁻³
 $\Delta\rho_{\min} = -0.37$ e Å⁻³
Table 1

Hydrogen-bond geometry (Å, °).

 C_g is the centroid of the C1/C2/C7/O1/C8 furan ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C12}-\text{H12A}\cdots\text{O3}^{\text{i}}$	0.99	2.52	3.493 (3)	166
$\text{C17}-\text{H17}\cdots\text{O3}^{\text{ii}}$	0.95	2.49	3.183 (3)	129
$\text{C10}-\text{H10B}\cdots\text{C}_g^{\text{iii}}$	0.99	2.68	3.604 (3)	156

 Symmetry codes: (i) $x + 1, -y + \frac{1}{2}, z - \frac{1}{2}$; (ii) $-x + 1, y - \frac{1}{2}, -z + \frac{3}{2}$; (iii) $x + 1, y, z$.

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.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2391).

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supporting information

Acta Cryst. (2011). E67, o2223 [doi:10.1107/S160053681103042X]

5-Cyclopentyl-2-methyl-3-phenylsulfonyl-1-benzofuran

Pil Ja Seo, Hong Dae Choi, Byeng Wha Son and Uk Lee

S1. Comment

Recently, many compounds involving a benzofuran skeleton have drawn much attention owing to their valuable pharmacological 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 continuing studies of the substituent effect on the solid state structures of 5-alkyl-2-methyl-3-phenylsulfonyl-1-benzofuran analogues (Choi *et al.*, 2008*a,b*; Seo *et al.*, 2011), 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 0.020 (2) Å from the least-squares plane defined by the nine constituent atoms. The cyclopentyl ring is in the envelope form. The dihedral angle formed by the phenyl ring and the mean plane of the benzofuran fragment is 81.40 (6)°. The molecular packing (Fig. 2) is stabilized by weak intermolecular C—H···O hydrogen bonds; the first one between a cyclopentyl H atom and the O atom of the sulfonyl group (Table 1; C12—H12A···O3ⁱ), and the second one between a phenyl H atom and the O atom of the sulfonyl group (Table 1; C17—H17···O3ⁱⁱ). The crystal packing (Fig. 3) is further stabilized by intermolecular C—H··· π interactions between a cyclopentyl H atom and the furan ring (Table 1; C10—H10B···Cgⁱⁱⁱ, Cg is the centroid of the C1/C2/C7/O1/C8 furan ring).

S2. Experimental

77% 3-chloroperoxybenzoic acid (448 mg, 2.0 mmol) was added in small portions to a stirred solution of 5-cyclopentyl-2-methyl-3-phenylsulfonyl-1-benzofuran (277 mg, 0.9 mmol) in dichloromethane (40 mL) at 273 K. After being stirred at room temperature for 8h, 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, 4:1 v/v) to afford the title compound as a colorless solid [yield 72%, m.p. 418–419 K; *R*_f = 0.48 (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.

S3. Refinement

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.95 Å for aryl, 1.00 Å for methine, 0.99 Å for methylene and 0.98 Å for methyl H atoms, respectively. $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for aryl, methine and methylene, and $1.5U_{\text{eq}}(\text{C})$ for methyl H atoms.

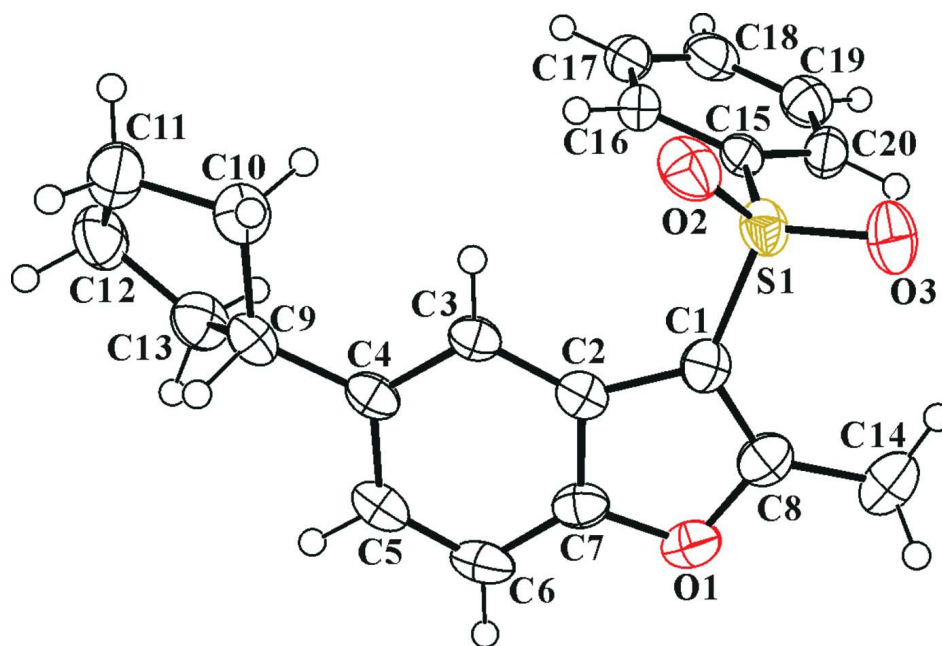


Figure 1

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.

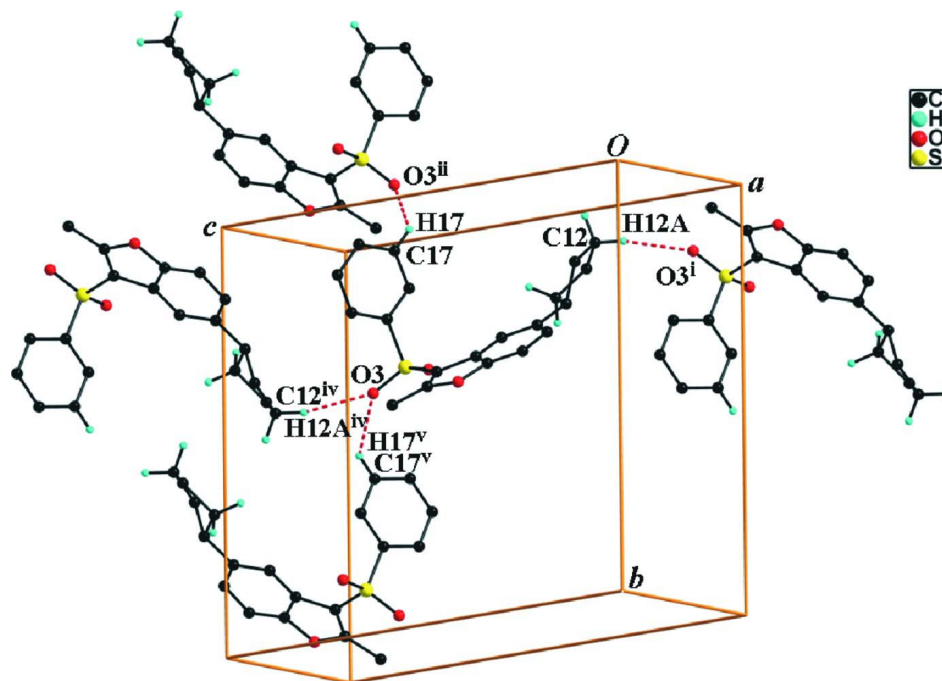
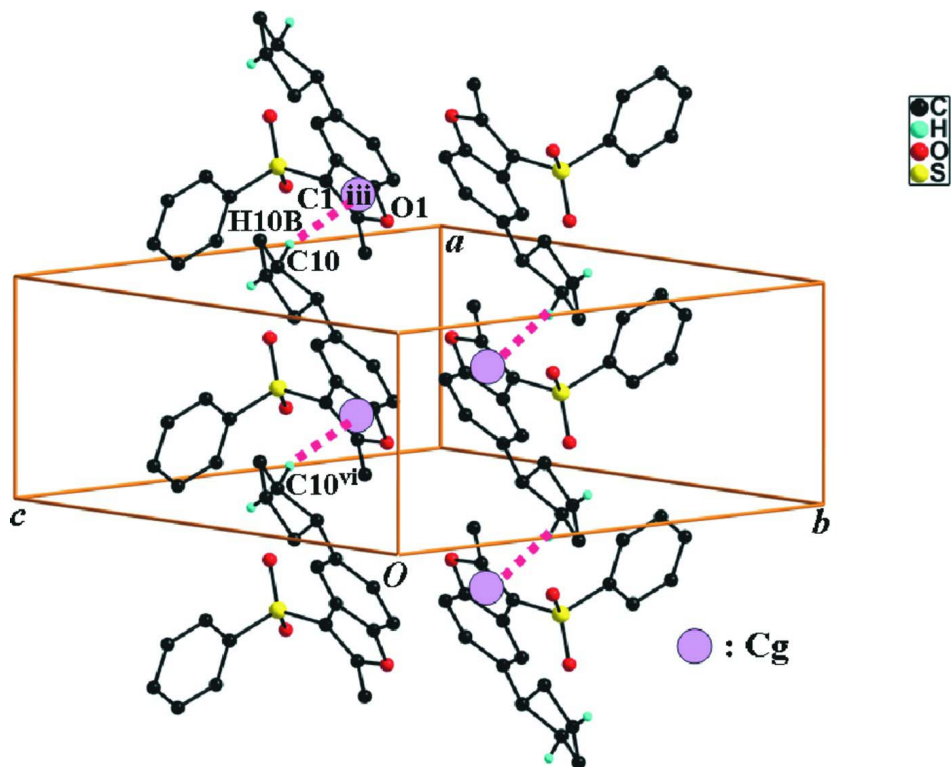


Figure 2

A view of the C—H...O interactions (dotted lines) in the crystal structure of the title compound. [Symmetry codes: (i) $x + 1, -y + 1/2, z - 1/2$; (ii) $-x + 1, y - 1/2, -z + 3/2$; (iv) $x - 1, -y + 1/2, z + 1/2$; (v) $-x + 1, y + 1/2, -z + 3/2$.]

**Figure 3**

A view of the C—H... π interactions (dotted lines) in the crystal structure of the title compound. [Symmetry codes: (iii) $x + 1, y, z$; (vi) $x - 1, y, z$.]

5-Cyclopentyl-2-methyl-3-phenylsulfonyl-1-benzofuran

Crystal data

$C_{20}H_{20}O_3S$

$M_r = 340.42$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

$a = 6.2999$ (9) Å

$b = 15.001$ (2) Å

$c = 17.743$ (2) Å

$\beta = 92.011$ (3)°

$V = 1675.8$ (4) Å³

$Z = 4$

$F(000) = 720$

$D_x = 1.349$ Mg m⁻³

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

Cell parameters from 3720 reflections

$\theta = 2.3$ – 25.9 °

$\mu = 0.21$ mm⁻¹

$T = 173$ K

Block, colourless

$0.27 \times 0.10 \times 0.08$ mm

Data collection

Bruker SMART APEXII CCD
diffractometer

Radiation source: rotating anode

Graphite multilayer monochromator

Detector resolution: 10.0 pixels mm⁻¹

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2009)

$T_{\min} = 0.946$, $T_{\max} = 0.983$

15497 measured reflections

3616 independent reflections

2869 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.065$

$\theta_{\max} = 27.0$ °, $\theta_{\min} = 1.8$ °

$h = -8 \rightarrow 8$

$k = -18 \rightarrow 19$

$l = -22 \rightarrow 22$

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.052$ $wR(F^2) = 0.130$ $S = 1.04$

3616 reflections

218 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

 $w = 1/[\sigma^2(F_o^2) + (0.0491P)^2 + 0.8019P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.44 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.37 \text{ e } \text{\AA}^{-3}$ *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 $F^2 > 2\sigma(F^2)$ 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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.49451 (8)	0.34441 (4)	0.69600 (3)	0.03570 (17)
O1	0.2815 (2)	0.42140 (10)	0.49705 (9)	0.0416 (4)
O2	0.7200 (2)	0.33502 (12)	0.70766 (9)	0.0469 (4)
O3	0.3805 (3)	0.40440 (11)	0.74236 (9)	0.0502 (4)
C1	0.4473 (3)	0.37248 (14)	0.60261 (12)	0.0337 (5)
C2	0.5648 (3)	0.33976 (13)	0.53954 (11)	0.0311 (4)
C3	0.7450 (3)	0.28710 (13)	0.53044 (11)	0.0304 (4)
H3	0.8255	0.2661	0.5731	0.036*
C4	0.8043 (3)	0.26593 (13)	0.45818 (11)	0.0312 (4)
C5	0.6835 (3)	0.29847 (15)	0.39625 (12)	0.0391 (5)
H5	0.7246	0.2829	0.3469	0.047*
C6	0.5081 (4)	0.35192 (16)	0.40378 (13)	0.0417 (5)
H6	0.4289	0.3742	0.3613	0.050*
C7	0.4540 (3)	0.37123 (14)	0.47631 (12)	0.0349 (5)
C8	0.2785 (3)	0.42026 (14)	0.57351 (13)	0.0380 (5)
C9	0.9944 (3)	0.20828 (14)	0.44394 (11)	0.0341 (5)
H9	1.0897	0.2426	0.4106	0.041*
C10	1.1282 (3)	0.17647 (15)	0.51169 (13)	0.0399 (5)
H10A	1.0380	0.1504	0.5506	0.048*
H10B	1.2124	0.2260	0.5343	0.048*
C11	1.2724 (4)	0.10590 (17)	0.47845 (15)	0.0503 (6)
H11A	1.3148	0.0610	0.5170	0.060*
H11B	1.4021	0.1336	0.4589	0.060*
C12	1.1391 (4)	0.06297 (18)	0.41446 (14)	0.0551 (7)
H12A	1.2193	0.0619	0.3675	0.066*

H12B	1.1012	0.0010	0.4277	0.066*
C13	0.9395 (4)	0.11989 (16)	0.40397 (13)	0.0463 (6)
H13A	0.8167	0.0908	0.4272	0.056*
H13B	0.9051	0.1299	0.3498	0.056*
C14	0.1001 (4)	0.46840 (16)	0.60728 (15)	0.0508 (6)
H14A	0.1019	0.5309	0.5914	0.076*
H14B	0.1147	0.4652	0.6624	0.076*
H14C	-0.0346	0.4410	0.5905	0.076*
C15	0.3793 (3)	0.23799 (14)	0.70462 (11)	0.0306 (4)
C16	0.4923 (4)	0.16333 (15)	0.68364 (12)	0.0397 (5)
H16	0.6306	0.1693	0.6645	0.048*
C17	0.4017 (4)	0.08023 (16)	0.69086 (13)	0.0484 (6)
H17	0.4779	0.0285	0.6769	0.058*
C18	0.2011 (4)	0.07225 (16)	0.71818 (13)	0.0475 (6)
H18	0.1400	0.0148	0.7235	0.057*
C19	0.0885 (4)	0.14626 (16)	0.73774 (13)	0.0438 (5)
H19	-0.0504	0.1399	0.7562	0.053*
C20	0.1760 (3)	0.23023 (15)	0.73080 (12)	0.0378 (5)
H20	0.0977	0.2818	0.7438	0.045*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0368 (3)	0.0405 (3)	0.0297 (3)	-0.0009 (2)	-0.0001 (2)	-0.0102 (2)
O1	0.0392 (8)	0.0379 (9)	0.0475 (10)	0.0027 (6)	-0.0034 (7)	0.0097 (7)
O2	0.0366 (8)	0.0688 (12)	0.0350 (9)	-0.0052 (7)	-0.0044 (6)	-0.0048 (8)
O3	0.0600 (10)	0.0460 (10)	0.0449 (10)	-0.0011 (8)	0.0077 (8)	-0.0213 (8)
C1	0.0347 (10)	0.0302 (10)	0.0361 (12)	-0.0023 (8)	0.0001 (9)	-0.0050 (9)
C2	0.0348 (10)	0.0296 (10)	0.0288 (11)	-0.0066 (8)	-0.0008 (8)	-0.0004 (8)
C3	0.0339 (10)	0.0318 (11)	0.0253 (10)	-0.0038 (8)	-0.0027 (8)	0.0015 (8)
C4	0.0347 (10)	0.0326 (11)	0.0262 (11)	-0.0109 (8)	0.0002 (8)	0.0023 (8)
C5	0.0450 (12)	0.0464 (13)	0.0260 (11)	-0.0102 (10)	0.0021 (9)	0.0043 (9)
C6	0.0433 (12)	0.0494 (14)	0.0318 (12)	-0.0079 (10)	-0.0067 (9)	0.0155 (10)
C7	0.0335 (10)	0.0320 (11)	0.0390 (12)	-0.0040 (8)	-0.0031 (9)	0.0077 (9)
C8	0.0380 (11)	0.0294 (11)	0.0465 (14)	-0.0032 (8)	-0.0009 (9)	-0.0003 (9)
C9	0.0387 (11)	0.0360 (11)	0.0280 (11)	-0.0076 (9)	0.0071 (9)	0.0003 (9)
C10	0.0380 (11)	0.0415 (13)	0.0402 (13)	-0.0051 (9)	-0.0004 (9)	-0.0068 (10)
C11	0.0436 (13)	0.0509 (15)	0.0569 (16)	0.0045 (11)	0.0083 (11)	-0.0020 (12)
C12	0.0709 (17)	0.0497 (15)	0.0459 (15)	0.0079 (12)	0.0178 (13)	-0.0066 (12)
C13	0.0574 (14)	0.0453 (14)	0.0360 (13)	-0.0031 (11)	-0.0001 (11)	-0.0090 (10)
C14	0.0413 (12)	0.0395 (13)	0.0715 (18)	0.0065 (10)	0.0017 (12)	-0.0011 (12)
C15	0.0343 (10)	0.0370 (11)	0.0201 (10)	0.0053 (8)	-0.0036 (8)	-0.0044 (8)
C16	0.0434 (12)	0.0450 (13)	0.0310 (12)	0.0156 (10)	0.0062 (9)	0.0021 (9)
C17	0.0731 (16)	0.0380 (13)	0.0345 (13)	0.0196 (11)	0.0065 (11)	0.0013 (10)
C18	0.0697 (16)	0.0392 (13)	0.0332 (13)	-0.0023 (11)	-0.0015 (11)	-0.0002 (10)
C19	0.0406 (12)	0.0512 (14)	0.0393 (13)	-0.0034 (10)	-0.0004 (10)	-0.0015 (10)
C20	0.0360 (11)	0.0413 (12)	0.0361 (12)	0.0076 (9)	0.0005 (9)	-0.0070 (9)

Geometric parameters (Å, °)

S1—O3	1.4295 (15)	C10—H10B	0.9900
S1—O2	1.4351 (16)	C11—C12	1.530 (4)
S1—C1	1.725 (2)	C11—H11A	0.9900
S1—C15	1.763 (2)	C11—H11B	0.9900
O1—C8	1.358 (3)	C12—C13	1.526 (3)
O1—C7	1.382 (3)	C12—H12A	0.9900
C1—C8	1.368 (3)	C12—H12B	0.9900
C1—C2	1.449 (3)	C13—H13A	0.9900
C2—C7	1.383 (3)	C13—H13B	0.9900
C2—C3	1.397 (3)	C14—H14A	0.9800
C3—C4	1.385 (3)	C14—H14B	0.9800
C3—H3	0.9500	C14—H14C	0.9800
C4—C5	1.402 (3)	C15—C20	1.383 (3)
C4—C9	1.506 (3)	C15—C16	1.385 (3)
C5—C6	1.376 (3)	C16—C17	1.379 (3)
C5—H5	0.9500	C16—H16	0.9500
C6—C7	1.374 (3)	C17—C18	1.374 (4)
C6—H6	0.9500	C17—H17	0.9500
C8—C14	1.481 (3)	C18—C19	1.369 (3)
C9—C10	1.520 (3)	C18—H18	0.9500
C9—C13	1.537 (3)	C19—C20	1.382 (3)
C9—H9	1.0000	C19—H19	0.9500
C10—C11	1.527 (3)	C20—H20	0.9500
C10—H10A	0.9900		
O3—S1—O2	119.56 (10)	C10—C11—C12	105.06 (19)
O3—S1—C1	109.02 (10)	C10—C11—H11A	110.7
O2—S1—C1	107.38 (10)	C12—C11—H11A	110.7
O3—S1—C15	107.67 (10)	C10—C11—H11B	110.7
O2—S1—C15	107.89 (10)	C12—C11—H11B	110.7
C1—S1—C15	104.29 (10)	H11A—C11—H11B	108.8
C8—O1—C7	107.31 (16)	C13—C12—C11	106.46 (19)
C8—C1—C2	107.29 (19)	C13—C12—H12A	110.4
C8—C1—S1	126.56 (17)	C11—C12—H12A	110.4
C2—C1—S1	125.71 (16)	C13—C12—H12B	110.4
C7—C2—C3	119.22 (19)	C11—C12—H12B	110.4
C7—C2—C1	104.71 (18)	H12A—C12—H12B	108.6
C3—C2—C1	136.06 (19)	C12—C13—C9	104.8 (2)
C4—C3—C2	118.90 (19)	C12—C13—H13A	110.8
C4—C3—H3	120.5	C9—C13—H13A	110.8
C2—C3—H3	120.5	C12—C13—H13B	110.8
C3—C4—C5	119.3 (2)	C9—C13—H13B	110.8
C3—C4—C9	121.93 (18)	H13A—C13—H13B	108.9
C5—C4—C9	118.78 (18)	C8—C14—H14A	109.5
C6—C5—C4	122.9 (2)	C8—C14—H14B	109.5
C6—C5—H5	118.6	H14A—C14—H14B	109.5

C4—C5—H5	118.6	C8—C14—H14C	109.5
C7—C6—C5	116.1 (2)	H14A—C14—H14C	109.5
C7—C6—H6	121.9	H14B—C14—H14C	109.5
C5—C6—H6	121.9	C20—C15—C16	120.9 (2)
C6—C7—O1	126.0 (2)	C20—C15—S1	119.64 (16)
C6—C7—C2	123.6 (2)	C16—C15—S1	119.45 (16)
O1—C7—C2	110.42 (18)	C17—C16—C15	119.2 (2)
O1—C8—C1	110.25 (19)	C17—C16—H16	120.4
O1—C8—C14	115.8 (2)	C15—C16—H16	120.4
C1—C8—C14	133.9 (2)	C18—C17—C16	120.0 (2)
C4—C9—C10	118.02 (17)	C18—C17—H17	120.0
C4—C9—C13	113.90 (17)	C16—C17—H17	120.0
C10—C9—C13	101.75 (18)	C19—C18—C17	120.6 (2)
C4—C9—H9	107.5	C19—C18—H18	119.7
C10—C9—H9	107.5	C17—C18—H18	119.7
C13—C9—H9	107.5	C18—C19—C20	120.3 (2)
C9—C10—C11	103.48 (18)	C18—C19—H19	119.8
C9—C10—H10A	111.1	C20—C19—H19	119.8
C11—C10—H10A	111.1	C19—C20—C15	118.9 (2)
C9—C10—H10B	111.1	C19—C20—H20	120.5
C11—C10—H10B	111.1	C15—C20—H20	120.5
H10A—C10—H10B	109.0		
O3—S1—C1—C8	-21.6 (2)	S1—C1—C8—O1	-173.51 (15)
O2—S1—C1—C8	-152.50 (19)	C2—C1—C8—C14	178.7 (2)
C15—S1—C1—C8	93.2 (2)	S1—C1—C8—C14	6.0 (4)
O3—S1—C1—C2	167.01 (17)	C3—C4—C9—C10	-2.7 (3)
O2—S1—C1—C2	36.1 (2)	C5—C4—C9—C10	177.77 (18)
C15—S1—C1—C2	-78.21 (19)	C3—C4—C9—C13	116.6 (2)
C8—C1—C2—C7	-0.1 (2)	C5—C4—C9—C13	-63.0 (2)
S1—C1—C2—C7	172.67 (15)	C4—C9—C10—C11	168.43 (18)
C8—C1—C2—C3	-178.6 (2)	C13—C9—C10—C11	43.0 (2)
S1—C1—C2—C3	-5.8 (3)	C9—C10—C11—C12	-32.8 (2)
C7—C2—C3—C4	-1.7 (3)	C10—C11—C12—C13	9.5 (3)
C1—C2—C3—C4	176.6 (2)	C11—C12—C13—C9	17.1 (3)
C2—C3—C4—C5	0.6 (3)	C4—C9—C13—C12	-165.15 (18)
C2—C3—C4—C9	-178.99 (17)	C10—C9—C13—C12	-37.1 (2)
C3—C4—C5—C6	0.8 (3)	O3—S1—C15—C20	19.5 (2)
C9—C4—C5—C6	-179.64 (19)	O2—S1—C15—C20	149.86 (17)
C4—C5—C6—C7	-0.9 (3)	C1—S1—C15—C20	-96.18 (18)
C5—C6—C7—O1	-178.17 (19)	O3—S1—C15—C16	-161.71 (17)
C5—C6—C7—C2	-0.3 (3)	O2—S1—C15—C16	-31.40 (19)
C8—O1—C7—C6	176.6 (2)	C1—S1—C15—C16	82.56 (18)
C8—O1—C7—C2	-1.5 (2)	C20—C15—C16—C17	-1.6 (3)
C3—C2—C7—C6	1.6 (3)	S1—C15—C16—C17	179.70 (17)
C1—C2—C7—C6	-177.2 (2)	C15—C16—C17—C18	0.4 (3)
C3—C2—C7—O1	179.78 (16)	C16—C17—C18—C19	0.7 (4)
C1—C2—C7—O1	1.0 (2)	C17—C18—C19—C20	-0.5 (4)

C7—O1—C8—C1	1.4 (2)	C18—C19—C20—C15	-0.7 (3)
C7—O1—C8—C14	-178.18 (18)	C16—C15—C20—C19	1.7 (3)
C2—C1—C8—O1	-0.8 (2)	S1—C15—C20—C19	-179.54 (17)

Hydrogen-bond geometry (Å, °)

Cg is the centroid of the C1/C2/C7/O1/C8 furan 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>
C12—H12 <i>A</i> ...O3 ⁱ	0.99	2.52	3.493 (3)	166
C17—H17...O3 ⁱⁱ	0.95	2.49	3.183 (3)	129
C10—H10 <i>B</i> ...Cg ⁱⁱⁱ	0.99	2.68	3.604 (3)	156

Symmetry codes: (i) $x+1, -y+1/2, z-1/2$; (ii) $-x+1, y-1/2, -z+3/2$; (iii) $x+1, y, z$.