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3-Cyclohexylsulfonyl-5-iodo-2,7-dimethyl-1-benzofuran

Pil Ja Seo,[a] Hong Dae Choi,[a] Byeng Wha Son[b] and Uk Lee[b]*

[a]Department of Chemistry, Dongeui University, San 24 Kaya-dong Busanjin-gu, Busan 614-714, Republic of Korea, and [b]Department 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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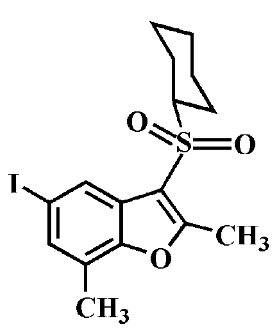
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.023; wR factor = 0.058; data-to-parameter ratio = 20.8.

In the title compound, $C_{16}H_{19}IO_3S$, the cyclohexyl ring adopts a chair conformation. In the crystal, pairs of intermolecular I···O contacts [3.269 (2) Å] link the molecules into inversion dimers. These dimers are further stabilized by a slipped π–π interaction between the benzene and furan rings of adjacent molecules [centroid–centroid distance = 3.701 (3) Å, interplanar distance = 3.372 (3) Å and slippage = 1.525 (3) Å].

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 3-cyclohexylsulfonyl-5-halo-2-methyl-1-benzofuran derivatives, see: Choi *et al.* (2011*a*,*b*,*c*). For a review on halogen bonding, see: Politzer *et al.* (2007).



Experimental

Crystal data

$C_{16}H_{19}IO_3S$
M_r = 418.27
Triclinic, $P\overline{1}$
a = 6.8643 (2) Å
b = 8.4981 (2) Å
c = 14.2323 (3) Å
α = 102.512 (1)°
β = 99.846 (1)°
γ = 92.092 (1)°
V = 796.23 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.15 mm^{-1}
T = 173 K
0.24 × 0.16 × 0.14 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.629, T_{max} = 0.759
15021 measured reflections
3997 independent reflections
3753 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.058
S = 1.06
3997 reflections
192 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.68 e Å^{-3}
$\Delta\rho_{min}$ = −0.63 e Å^{-3}

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: ZL2384).

References

Akgul, Y. Y. & Anil, H. (2003). *Phytochemistry*, **63**, 939–943.
Aslam, S. N., Stevenson, P. C., Kokubun, T. & Hall, D. R. (2009). *Microbiol. Res.* **164**, 191–195.
Brandenburg, K. (1998). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2009). *APEX2*, *SADABS* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Choi, H. D., Seo, P. J., Son, B. W. & Lee, U. (2011*a*). *Acta Cryst.* E**67**, o542.
Choi, H. D., Seo, P. J., Son, B. W. & Lee, U. (2011*b*). *Acta Cryst.* E**67**, o828.
Choi, H. D., Seo, P. J., Son, B. W. & Lee, U. (2011*c*). *Acta Cryst.* E**67**, o847.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Galal, S. A., Abd El-All, A. S., Abdallah, M. M. & El-Diwani, H. I. (2009). *Bioorg. Med. Chem. Lett.* **19**, 2420–2428.
Khan, M. W., Alam, M. J., Rashid, M. A. & Chowdhury, R. (2005). *Bioorg. Med. Chem.* **13**, 4796–4805.
Politzer, P., Lane, P., Concha, M. C., Ma, Y. & Murray, J. S. (2007). *J. Mol. Model.* **13**, 305–311.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Soekamto, N. H., Achmad, S. A., Ghisalberti, E. L., Hakim, E. H. & Syah, Y. M. (2003). *Phytochemistry*, **64**, 831–834.

supporting information

Acta Cryst. (2011). E**67**, o2053   [doi:10.1107/S1600536811027395]

3-Cyclohexylsulfonyl-5-iodo-2,7-dimethyl-1-benzofuran

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S1. Comment

Recently, many compounds containing a benzofuran moiety 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 ongoing study of the substituent effect on the solid state structures of 3-cyclohexylsulfonyl-5-halo-2-methyl-1-benzofuran analogues (Choi *et al.*, 2011*a,b,c*), 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 0.007 (2) Å from the least-squares plane defined by the nine constituent atoms. The cyclohexyl ring is in the chair form. The molecular packing (Fig. 2) is stabilized by I···O halogen-bondings between the iodine and the O atom of the sulfonyl group [I1···O2^{ii} = 3.269 (2) Å; C4—11···O2^{ii} = 168.48 (6)°] (Politzer *et al.*, 2007). The crystal packing (Fig. 2) is further stabilized by a weak slipped $\pi\cdots\pi$ interaction between the benzene and furan rings of adjacent molecules, with a Cg1···Cg2^{i} distance of 3.701 (3) Å and an interplanar distance of 3.372 (3) Å resulting in a slippage of 1.525 (3) Å (Cg1 and Cg2 are the centroids of the C2–C7 benzene ring and the C1/C2/C7/O1/C8 furan ring, respectively, see Fig. 2 for symmetry codes).

S2. Experimental

77% 3-chloroperoxybenzoic acid (426 mg, 1.9 mmol) was added in small portions to a stirred solution of 3-cyclohexyl-sulfanyl-5-iodo-2,7-dimethyl-1-benzofuran (347 mg, 0.9 mmol) in dichloromethane (35 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 71%, m.p. 441–442 K; R_f = 0.63 (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_{iso}(H) = 1.2U_{eq}(C) for aryl, methine and methylene, and 1.5U_{eq}(C) for methyl H atoms.

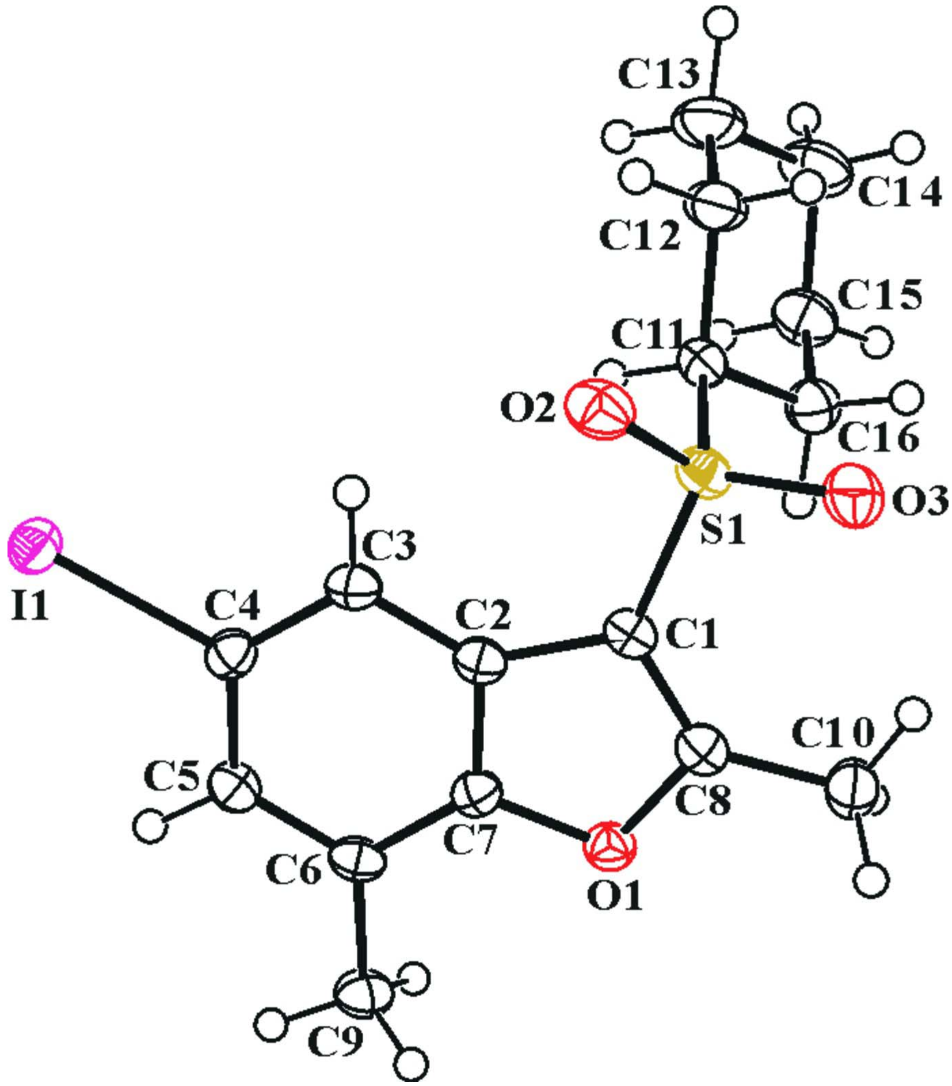

Figure 1

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 a small spheres of arbitrary radius.

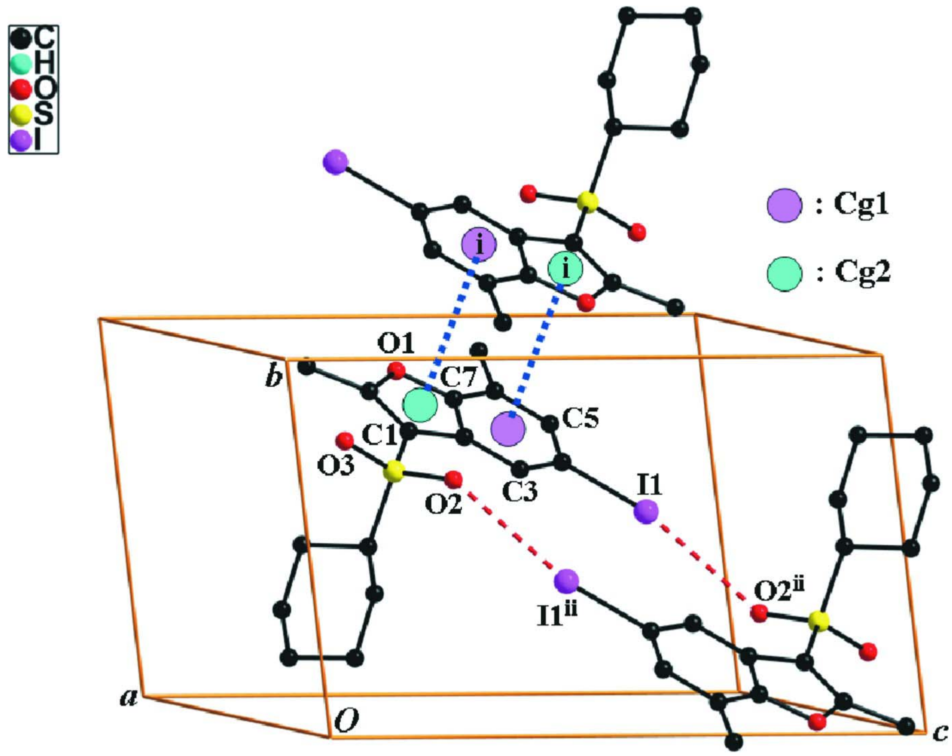

Figure 2

A view of the I···O and $\pi\cdots\pi$ interactions (dotted lines) in the crystal structure of the title compound. [Symmetry codes: (i) - *x* + 1, - *y* + 2, - *z* + 1; (ii) - *x*, - *y* + 1, - *z* + 1.]

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Crystal data

$C_{16}H_{19}IO_3S$
M_r = 418.27
Triclinic, $P\bar{1}$
Hall symbol: -P 1
a = 6.8643 (2) Å
b = 8.4981 (2) Å
c = 14.2323 (3) Å
α = 102.512 (1)°
β = 99.846 (1)°
γ = 92.092 (1)°
V = 796.23 (3) Å^3
Z = 2
F(000) = 416
D_x = 1.745 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 8926 reflections
θ = 2.5–28.4°
μ = 2.15 mm^{-1}
T = 173 K
Block, colourless
0.24 × 0.16 × 0.14 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} = 0.629, T_{max} = 0.759
15021 measured reflections
3997 independent reflections
3753 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 28.4°, θ_{min} = 1.5°
h = −7→9
k = −11→11
l = −19→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.058$
$S = 1.06$
3997 reflections
192 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0291P)^2 + 0.2895P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 0.68$ e Å^{-3}
$\Delta\rho_{min} = -0.63$ e Å^{-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 > 2sigma(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}
I1	0.227778 (18)	0.565947 (15)	0.643317 (9)	0.02648 (5)
S1	0.19017 (7)	0.68116 (6)	0.21668 (4)	0.02476 (10)
O1	0.6820 (2)	0.89122 (16)	0.38987 (10)	0.0237 (3)
O2	0.0181 (2)	0.67742 (19)	0.26177 (12)	0.0329 (3)
O3	0.1832 (3)	0.76329 (19)	0.13777 (12)	0.0350 (4)
C1	0.3897 (3)	0.7652 (2)	0.30960 (14)	0.0224 (4)
C2	0.4132 (3)	0.7461 (2)	0.40933 (14)	0.0211 (4)
C3	0.3023 (3)	0.6713 (2)	0.46236 (14)	0.0234 (4)
H3	0.1761	0.6163	0.4336	0.028*
C4	0.3852 (3)	0.6808 (2)	0.55982 (14)	0.0229 (4)
C5	0.5707 (3)	0.7612 (2)	0.60332 (14)	0.0231 (4)
H5	0.6207	0.7642	0.6702	0.028*
C6	0.6829 (3)	0.8363 (2)	0.55159 (15)	0.0225 (4)
C7	0.5962 (3)	0.8262 (2)	0.45489 (14)	0.0211 (4)
C8	0.5545 (3)	0.8523 (2)	0.30207 (14)	0.0238 (4)
C9	0.8856 (3)	0.9191 (3)	0.59487 (16)	0.0278 (4)
H9A	0.9151	0.9214	0.6650	0.042*
H9B	0.8892	1.0300	0.5855	0.042*
H9C	0.9846	0.8600	0.5623	0.042*
C10	0.6225 (3)	0.9118 (3)	0.22258 (16)	0.0311 (4)
H10A	0.6478	1.0297	0.2421	0.047*
H10B	0.5201	0.8827	0.1633	0.047*
H10C	0.7449	0.8628	0.2094	0.047*
C11	0.2463 (3)	0.4764 (2)	0.17566 (14)	0.0252 (4)
H11	0.2952	0.4337	0.2349	0.030*

C12	0.0574 (3)	0.3736 (3)	0.11981 (17)	0.0342 (5)
H12A	−0.0438	0.3806	0.1622	0.041*
H12B	0.0030	0.4145	0.0614	0.041*
C13	0.1052 (4)	0.1980 (3)	0.0884 (2)	0.0461 (6)
H13A	0.1485	0.1550	0.1473	0.055*
H13B	−0.0160	0.1324	0.0500	0.055*
C14	0.2662 (4)	0.1825 (3)	0.0274 (2)	0.0446 (6)
H14A	0.2180	0.2151	−0.0346	0.054*
H14B	0.2979	0.0681	0.0112	0.054*
C15	0.4538 (4)	0.2879 (3)	0.08190 (18)	0.0365 (5)
H15A	0.5530	0.2811	0.0385	0.044*
H15B	0.5111	0.2470	0.1399	0.044*
C16	0.4094 (3)	0.4643 (3)	0.11478 (16)	0.0303 (4)
H16A	0.5310	0.5283	0.1541	0.036*
H16B	0.3672	0.5096	0.0567	0.036*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.02413 (8)	0.02921 (8)	0.02755 (8)	0.00073 (5)	0.00534 (5)	0.00927 (5)
S1	0.0237 (2)	0.0259 (2)	0.0223 (2)	0.00194 (18)	−0.00089 (18)	0.00417 (18)
O1	0.0210 (7)	0.0248 (7)	0.0242 (7)	−0.0001 (5)	0.0038 (5)	0.0039 (5)
O2	0.0221 (7)	0.0389 (9)	0.0338 (8)	0.0025 (6)	0.0019 (6)	0.0022 (6)
O3	0.0392 (9)	0.0337 (8)	0.0312 (8)	0.0025 (7)	−0.0044 (7)	0.0138 (6)
C1	0.0218 (9)	0.0223 (9)	0.0211 (9)	0.0025 (7)	0.0017 (7)	0.0024 (7)
C2	0.0201 (9)	0.0189 (8)	0.0227 (9)	0.0030 (7)	0.0030 (7)	0.0020 (7)
C3	0.0197 (9)	0.0227 (9)	0.0256 (9)	−0.0006 (7)	0.0022 (7)	0.0024 (7)
C4	0.0226 (9)	0.0216 (9)	0.0254 (9)	0.0019 (7)	0.0064 (7)	0.0054 (7)
C5	0.0224 (9)	0.0237 (9)	0.0224 (9)	0.0041 (7)	0.0017 (7)	0.0046 (7)
C6	0.0204 (9)	0.0183 (8)	0.0257 (9)	0.0030 (7)	0.0009 (7)	0.0010 (7)
C7	0.0206 (9)	0.0189 (8)	0.0239 (9)	0.0021 (7)	0.0056 (7)	0.0039 (7)
C8	0.0249 (9)	0.0223 (9)	0.0230 (9)	0.0046 (7)	0.0025 (7)	0.0036 (7)
C9	0.0202 (9)	0.0300 (10)	0.0302 (10)	−0.0015 (8)	−0.0014 (8)	0.0054 (8)
C10	0.0329 (11)	0.0346 (11)	0.0277 (10)	0.0014 (9)	0.0071 (9)	0.0100 (8)
C11	0.0289 (10)	0.0245 (9)	0.0203 (9)	−0.0009 (8)	0.0019 (8)	0.0036 (7)
C12	0.0302 (11)	0.0368 (12)	0.0294 (11)	−0.0073 (9)	0.0045 (9)	−0.0034 (9)
C13	0.0499 (16)	0.0352 (13)	0.0436 (14)	−0.0134 (11)	0.0089 (12)	−0.0092 (10)
C14	0.0479 (15)	0.0363 (13)	0.0398 (13)	−0.0014 (11)	0.0066 (11)	−0.0106 (10)
C15	0.0369 (13)	0.0331 (12)	0.0353 (12)	0.0053 (9)	0.0057 (10)	−0.0009 (9)
C16	0.0304 (11)	0.0312 (11)	0.0286 (10)	0.0011 (8)	0.0068 (9)	0.0047 (8)

Geometric parameters (Å, º)

I1—C4	2.097 (2)	C9—H9C	0.9800
I1—O2^{i}	3.2688 (17)	C10—H10A	0.9800
S1—O2	1.4401 (17)	C10—H10B	0.9800
S1—O3	1.4403 (16)	C10—H10C	0.9800
S1—C1	1.742 (2)	C11—C16	1.522 (3)

S1—C11	1.790 (2)	C11—C12	1.530 (3)
O1—C8	1.365 (2)	C11—H11	1.0000
O1—C7	1.376 (2)	C12—C13	1.527 (3)
C1—C8	1.361 (3)	C12—H12A	0.9900
C1—C2	1.446 (3)	C12—H12B	0.9900
C2—C3	1.386 (3)	C13—C14	1.510 (4)
C2—C7	1.389 (3)	C13—H13A	0.9900
C3—C4	1.390 (3)	C13—H13B	0.9900
C3—H3	0.9500	C14—C15	1.528 (3)
C4—C5	1.398 (3)	C14—H14A	0.9900
C5—C6	1.380 (3)	C14—H14B	0.9900
C5—H5	0.9500	C15—C16	1.529 (3)
C6—C7	1.386 (3)	C15—H15A	0.9900
C6—C9	1.503 (3)	C15—H15B	0.9900
C8—C10	1.472 (3)	C16—H16A	0.9900
C9—H9A	0.9800	C16—H16B	0.9900
C9—H9B	0.9800		

C4—I1—O2^{i}	168.48 (6)	H10A—C10—H10B	109.5
O2—S1—O3	118.27 (10)	C8—C10—H10C	109.5
O2—S1—C1	107.00 (9)	H10A—C10—H10C	109.5
O3—S1—C1	109.53 (10)	H10B—C10—H10C	109.5
O2—S1—C11	107.41 (10)	C16—C11—C12	111.79 (17)
O3—S1—C11	109.40 (10)	C16—C11—S1	111.94 (14)
C1—S1—C11	104.32 (9)	C12—C11—S1	109.81 (15)
C8—O1—C7	107.13 (15)	C16—C11—H11	107.7
C8—C1—C2	107.46 (17)	C12—C11—H11	107.7
C8—C1—S1	127.49 (16)	S1—C11—H11	107.7
C2—C1—S1	124.98 (15)	C13—C12—C11	109.4 (2)
C3—C2—C7	119.59 (18)	C13—C12—H12A	109.8
C3—C2—C1	135.79 (18)	C11—C12—H12A	109.8
C7—C2—C1	104.61 (17)	C13—C12—H12B	109.8
C2—C3—C4	116.60 (18)	C11—C12—H12B	109.8
C2—C3—H3	121.7	H12A—C12—H12B	108.2
C4—C3—H3	121.7	C14—C13—C12	111.6 (2)
C3—C4—C5	122.42 (19)	C14—C13—H13A	109.3
C3—C4—I1	118.52 (14)	C12—C13—H13A	109.3
C5—C4—I1	119.05 (14)	C14—C13—H13B	109.3
C6—C5—C4	121.71 (18)	C12—C13—H13B	109.3
C6—C5—H5	119.1	H13A—C13—H13B	108.0
C4—C5—H5	119.1	C13—C14—C15	111.3 (2)
C5—C6—C7	114.71 (17)	C13—C14—H14A	109.4
C5—C6—C9	123.24 (19)	C15—C14—H14A	109.4
C7—C6—C9	122.03 (19)	C13—C14—H14B	109.4
O1—C7—C6	124.57 (17)	C15—C14—H14B	109.4
O1—C7—C2	110.47 (16)	H14A—C14—H14B	108.0
C6—C7—C2	124.95 (19)	C14—C15—C16	111.3 (2)
C1—C8—O1	110.33 (17)	C14—C15—H15A	109.4

C1—C8—C10	134.78 (19)	C16—C15—H15A	109.4
O1—C8—C10	114.89 (18)	C14—C15—H15B	109.4
C6—C9—H9A	109.5	C16—C15—H15B	109.4
C6—C9—H9B	109.5	H15A—C15—H15B	108.0
H9A—C9—H9B	109.5	C11—C16—C15	110.27 (19)
C6—C9—H9C	109.5	C11—C16—H16A	109.6
H9A—C9—H9C	109.5	C15—C16—H16A	109.6
H9B—C9—H9C	109.5	C11—C16—H16B	109.6
C8—C10—H10A	109.5	C15—C16—H16B	109.6
C8—C10—H10B	109.5	H16A—C16—H16B	108.1

O2—S1—C1—C8	−150.57 (18)	C9—C6—C7—C2	177.36 (18)
O3—S1—C1—C8	−21.2 (2)	C3—C2—C7—O1	179.81 (16)
C11—S1—C1—C8	95.78 (19)	C1—C2—C7—O1	0.2 (2)
O2—S1—C1—C2	32.94 (19)	C3—C2—C7—C6	1.2 (3)
O3—S1—C1—C2	162.28 (16)	C1—C2—C7—C6	−178.46 (18)
C11—S1—C1—C2	−80.70 (18)	C2—C1—C8—O1	−0.2 (2)
C8—C1—C2—C3	−179.5 (2)	S1—C1—C8—O1	−177.21 (14)
S1—C1—C2—C3	−2.4 (3)	C2—C1—C8—C10	179.9 (2)
C8—C1—C2—C7	0.0 (2)	S1—C1—C8—C10	2.9 (4)
S1—C1—C2—C7	177.11 (14)	C7—O1—C8—C1	0.3 (2)
C7—C2—C3—C4	−0.5 (3)	C7—O1—C8—C10	−179.77 (16)
C1—C2—C3—C4	179.0 (2)	O2—S1—C11—C16	172.45 (14)
C2—C3—C4—C5	0.0 (3)	O3—S1—C11—C16	42.91 (17)
C2—C3—C4—I1	−178.70 (13)	C1—S1—C11—C16	−74.20 (16)
O2^{i}—I1—C4—C3	54.4 (4)	O2—S1—C11—C12	47.67 (17)
O2^{i}—I1—C4—C5	−124.3 (3)	O3—S1—C11—C12	−81.87 (17)
C3—C4—C5—C6	0.0 (3)	C1—S1—C11—C12	161.02 (15)
I1—C4—C5—C6	178.69 (14)	C16—C11—C12—C13	57.2 (3)
C4—C5—C6—C7	0.5 (3)	S1—C11—C12—C13	−177.91 (17)
C4—C5—C6—C9	−177.95 (18)	C11—C12—C13—C14	−56.7 (3)
C8—O1—C7—C6	178.33 (18)	C12—C13—C14—C15	56.3 (3)
C8—O1—C7—C2	−0.3 (2)	C13—C14—C15—C16	−55.2 (3)
C5—C6—C7—O1	−179.56 (17)	C12—C11—C16—C15	−56.8 (2)
C9—C6—C7—O1	−1.1 (3)	S1—C11—C16—C15	179.57 (15)
C5—C6—C7—C2	−1.1 (3)	C14—C15—C16—C11	55.0 (3)

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