

## 2-(4-Bromophenyl)-5-fluoro-3-phenylsulfanyl-1-benzofuran

Hong Dae Choi,<sup>a</sup> Pil Ja Seo,<sup>a</sup> Byung Wha Son<sup>b</sup> and Uk Lee<sup>b\*</sup>

<sup>a</sup>Department of Chemistry, Donggeui University, San 24 Kaya-dong Busanjin-gu, Busan 614-714, Republic of Korea, and <sup>b</sup>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

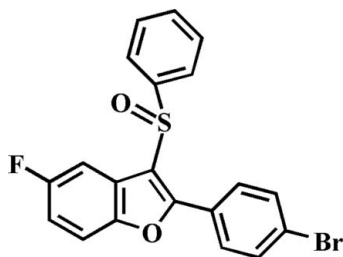
Received 14 July 2010; accepted 28 July 2010

Key indicators: single-crystal X-ray study;  $T = 173$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.030;  $wR$  factor = 0.104; data-to-parameter ratio = 17.0.

In the title compound,  $\text{C}_{20}\text{H}_{12}\text{BrFO}_2\text{S}$ , the O atom and the phenyl group of the phenylsulfanyl substituent lie on opposite sides of the plane through the benzofuran fragment; the phenyl ring is nearly perpendicular to this plane [dihedral angle =  $86.98$  (6)°]. The 4-bromophenyl ring is rotated slightly out of the benzofuran plane, making a dihedral angle of  $1.56$  (8)°. The crystal structure features aromatic  $\pi$ - $\pi$  interactions between the furan and phenyl rings of neighbouring molecules [centroid-centroid distance =  $3.506$  (3) Å], and an intermolecular  $\text{C}-\text{H}\cdots\pi$  interaction. The crystal structure also exhibits a short intermolecular  $\text{S}\cdots\text{S}$  contact [ $3.2635$  (8) Å].

### Related literature

For the pharmacological activity of benzofuran compounds, see: Aslam *et al.* (2006); Galal *et al.* (2009); Khan *et al.* (2005). For natural products with benzofuran rings, see: Akgul & Anil (2003); Soekamto *et al.* (2003). For the structures of related 5-halo-2-phenyl-3-phenylsulfanyl-1-benzofuran derivatives, see: Choi *et al.* (2009a,b,c). For short  $\text{S}\cdots\text{S}$  interactions, see: Munshi & Guru Row (2004).



### Experimental

#### Crystal data

$\text{C}_{20}\text{H}_{12}\text{BrFO}_2\text{S}$	$\gamma = 69.155$ (2)°
$M_r = 415.27$	$V = 829.78$ (7) Å <sup>3</sup>
Triclinic, $P\bar{1}$	$Z = 2$
$a = 8.1361$ (4) Å	Mo $K\alpha$ radiation
$b = 9.8237$ (5) Å	$\mu = 2.62$ mm <sup>-1</sup>
$c = 11.4093$ (5) Å	$T = 173$ K
$\alpha = 82.866$ (3)°	$0.29 \times 0.26 \times 0.21$ mm
$\beta = 77.123$ (3)°	

#### Data collection

Bruker SMART APEXII CCD diffractometer	14582 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2009)	3833 independent reflections
$T_{\min} = 0.664$ , $T_{\max} = 0.746$	3452 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.033$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.030$	226 parameters
$wR(F^2) = 0.104$	H-atom parameters constrained
$S = 0.87$	$\Delta\rho_{\text{max}} = 0.37$ e Å <sup>-3</sup>
3833 reflections	$\Delta\rho_{\text{min}} = -0.63$ e Å <sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

Cg3 is the centroid of the C15–C20 phenyl ring.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C5}-\text{H5}\cdots\text{Cg3}^i$	0.93	2.85	3.644 (3)	145

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

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: PK2256).

### References

- Akgul, Y. Y. & Anil, H. (2003). *Phytochemistry*, **63**, 939–943.  
 Aslam, S. N., Stevenson, P. C., Phythian, S. J., Veitch, N. C. & Hall, D. R. (2006). *Tetrahedron*, **62**, 4214–4226.  
 Brandenburg, K. (1998). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.  
 Bruker (2009). *APEX2*. *SADABS* and *SAINTE*. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Choi, H. D., Seo, P. J., Son, B. W. & Lee, U. (2009a). *Acta Cryst.* **E65**, o1809.  
 Choi, H. D., Seo, P. J., Son, B. W. & Lee, U. (2009b). *Acta Cryst.* **E65**, o1958.  
 Choi, H. D., Seo, P. J., Son, B. W. & Lee, U. (2009c). *Acta Cryst.* **E65**, o2609.  
 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.  
 Munshi, P. & Guru Row, T. N. (2004). *Acta Cryst.* **E60**, o2168–o2170.  
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
 Soekamto, N. H., Achmad, S. A., Ghisalberti, E. L., Hakim, E. H. & Syah, Y. M. (2003). *Phytochemistry*, **64**, 831–834.

**supplementary materials**

*Acta Cryst.* (2010). E66, o2172 [ doi:10.1107/S1600536810029958 ]

## 2-(4-Bromophenyl)-5-fluoro-3-phenylsulfinyl-1-benzofuran

H. D. Choi, P. J. Seo, B. W. Son and U. Lee

### Comment

Many compounds containing a benzofuran moiety have attracted considerable interest in view of their pharmacological properties such as antifungal, antitumor and antiviral, antimicrobial activities (Aslam *et al.*, 2006, Galal *et al.*, 2009, Khan *et al.*, 2005). These compounds occur widely in nature (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-halo-2-phenyl-3-phenylsulfinyl-1-benzofuran analogues (Choi *et al.*, 2009*a,b,c*), we report the crystal structure of the title compound (Fig. 1).

The benzofuran unit is essentially planar, with a mean deviation of 0.063 (1) Å from the least-squares plane defined by the nine constituent atoms. The dihedral angle formed by the benzofuran plane and the phenyl ring is 86.98 (6)°, and the 4-bromophenyl ring with 1.56 (8)° lies toward the benzofuran plane. The crystal packing (Fig. 2) is stabilized by aromatic  $\pi$ - $\pi$  interactions between the furan and benzene rings of the adjacent molecules, with a Cg1 $\cdots$ Cg2<sup>ii</sup> distance of 3.506 (3) Å (Cg1 and Cg2 are the centroids of the C1/C2/C7/O1/C8 furan ring and the C2-C7 benzene ring, respectively). The molecular packing (Fig. 2) is further stabilized by an intermolecular C—H $\cdots$  $\pi$  interaction between the benzene H atom and the phenyl ring of a neighbouring molecule, with a C5—H5 $\cdots$ Cg3<sup>i</sup> (Table 1; Cg3 is the centroid of the C15-C20 phenyl ring). The crystal structure also exhibits a short intermolecular S $\cdots$ S contact (Munshi & Guru Row, 2004), with a S $\cdots$ S<sup>iv</sup> distance of 3.2635 (8) Å.

### Experimental

77% 3-chloroperoxybenzoic acid (247 mg, 1.1 mmol) was added in small portions to a stirred solution of 2-(4-bromophenyl)-5-fluoro-3-phenylsulfonyl-1-benzofuran (439 mg, 0.8 mmol) in dichloromethane (40 mL) at 273 K. After being stirred at room temperature for 6h, 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 68%, m.p. 465–466 K;  $R_f$  = 0.75 (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 benzene at room temperature.

### Refinement

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å and  $U_{iso}(H) = 1.2U_{eq}(C)$ .

## Figures

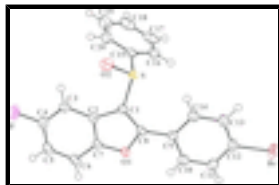


Fig. 1. The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are presented as a small spheres of arbitrary radius.

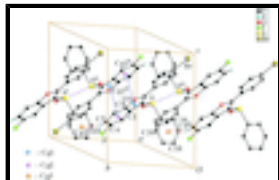


Fig. 2.  $\pi$ - $\pi$ , C—H $\cdots\pi$  and S $\cdots$ S interactions (dotted lines) in the crystal structure of the title compound. Cg denotes the ring centroids. [Symmetry codes: (i)  $x, y + 1, z$ ; (ii)  $-x + 1, -y + 1, -z + 1$ ; (iii)  $x, y - 1, z$ ; (iv)  $-x + 1, -y, -z + 1$ .]

## 2-(4-Bromophenyl)-5-fluoro-3-phenylsulfinyl-1-benzofuran

### Crystal data

$C_{20}H_{12}BrFO_2S$

$M_r = 415.27$

Triclinic,  $P\bar{1}$

Hall symbol: -P 1

$a = 8.1361$  (4) Å

$b = 9.8237$  (5) Å

$c = 11.4093$  (5) Å

$\alpha = 82.866$  (3)°

$\beta = 77.123$  (3)°

$\gamma = 69.155$  (2)°

$V = 829.78$  (7) Å<sup>3</sup>

$Z = 2$

$F(000) = 416$

$D_x = 1.662$  Mg m<sup>-3</sup>

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

Cell parameters from 8238 reflections

$\theta = 2.7$ – $27.5$ °

$\mu = 2.62$  mm<sup>-1</sup>

$T = 173$  K

Block, colourless

$0.29 \times 0.26 \times 0.21$  mm

### Data collection

Bruker SMART APEXII CCD diffractometer

Radiation source: rotating anode graphite multilayer

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

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan (SADABS; Bruker, 2009)

$T_{\min} = 0.664$ ,  $T_{\max} = 0.746$

14582 measured reflections

3833 independent reflections

3452 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.033$

$\theta_{\max} = 27.6$ °,  $\theta_{\min} = 1.8$ °

$h = -10 \rightarrow 10$

$k = -12 \rightarrow 12$

$l = -14 \rightarrow 14$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

$$R[F^2 > 2\sigma(F^2)] = 0.030$$

$$wR(F^2) = 0.104$$

$$S = 0.87$$

3833 reflections

226 parameters

0 restraints

Hydrogen site location: difference Fourier map

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.001$$

$$\Delta\rho_{\max} = 0.37 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.63 \text{ e } \text{\AA}^{-3}$$

### 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 ( $\text{\AA}^2$ )

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Br	-0.21990 (3)	0.22528 (2)	0.998902 (16)	0.03781 (11)
S	0.47916 (5)	0.16534 (4)	0.44461 (4)	0.02033 (12)
F	0.64982 (17)	0.61956 (15)	0.12311 (11)	0.0381 (3)
O1	0.17961 (16)	0.57103 (13)	0.53100 (11)	0.0210 (3)
O2	0.66591 (17)	0.14226 (15)	0.37795 (13)	0.0302 (3)
C1	0.3705 (2)	0.35537 (18)	0.46114 (14)	0.0193 (3)
C2	0.4126 (2)	0.46848 (19)	0.37985 (15)	0.0196 (3)
C3	0.5388 (2)	0.4728 (2)	0.27522 (16)	0.0238 (4)
H3	0.6234	0.3885	0.2413	0.029*
C4	0.5298 (2)	0.6096 (2)	0.22567 (16)	0.0264 (4)
C5	0.4074 (3)	0.7387 (2)	0.27342 (17)	0.0280 (4)
H5	0.4087	0.8278	0.2353	0.034*
C6	0.2835 (2)	0.7350 (2)	0.37772 (16)	0.0245 (4)
H6	0.2004	0.8197	0.4121	0.029*
C7	0.2906 (2)	0.59795 (19)	0.42783 (15)	0.0201 (3)
C8	0.2314 (2)	0.42188 (17)	0.55135 (15)	0.0191 (3)
C9	0.1288 (2)	0.37299 (19)	0.65891 (15)	0.0203 (3)
C10	-0.0123 (3)	0.4752 (2)	0.73078 (17)	0.0273 (4)
H10	-0.0387	0.5740	0.7092	0.033*
C11	-0.1131 (3)	0.4322 (2)	0.83305 (18)	0.0307 (4)
H11	-0.2057	0.5011	0.8804	0.037*
C12	-0.0740 (2)	0.2854 (2)	0.86369 (16)	0.0256 (4)
C13	0.0653 (3)	0.1814 (2)	0.79636 (17)	0.0293 (4)
H13	0.0911	0.0830	0.8194	0.035*

## supplementary materials

---

C14	0.1662 (3)	0.2245 (2)	0.69446 (17)	0.0275 (4)
H14	0.2600	0.1546	0.6488	0.033*
C15	0.3563 (2)	0.14738 (19)	0.33775 (17)	0.0217 (3)
C16	0.1896 (2)	0.1320 (2)	0.37783 (19)	0.0289 (4)
H16	0.1418	0.1280	0.4597	0.035*
C17	0.0958 (3)	0.1228 (2)	0.2932 (2)	0.0396 (5)
H17	-0.0171	0.1142	0.3183	0.047*
C18	0.1684 (3)	0.1263 (2)	0.1723 (2)	0.0432 (6)
H18	0.1041	0.1204	0.1164	0.052*
C19	0.3370 (4)	0.1387 (3)	0.1332 (2)	0.0461 (6)
H19	0.3856	0.1406	0.0514	0.055*
C20	0.4327 (3)	0.1481 (2)	0.21686 (18)	0.0347 (5)
H20	0.5465	0.1549	0.1918	0.042*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Br	0.03745 (16)	0.05065 (18)	0.02458 (14)	-0.02139 (12)	0.00266 (9)	0.00468 (10)
S	0.0185 (2)	0.0151 (2)	0.0247 (2)	-0.00334 (16)	-0.00247 (16)	-0.00170 (16)
F	0.0399 (7)	0.0428 (7)	0.0292 (6)	-0.0205 (6)	0.0043 (5)	0.0072 (5)
O1	0.0219 (6)	0.0140 (6)	0.0237 (6)	-0.0041 (5)	-0.0017 (5)	0.0004 (4)
O2	0.0171 (6)	0.0280 (7)	0.0422 (8)	-0.0040 (5)	-0.0009 (5)	-0.0096 (6)
C1	0.0199 (8)	0.0158 (8)	0.0213 (8)	-0.0059 (6)	-0.0031 (6)	0.0000 (6)
C2	0.0205 (8)	0.0188 (8)	0.0211 (8)	-0.0085 (7)	-0.0054 (6)	0.0007 (6)
C3	0.0226 (8)	0.0260 (9)	0.0225 (8)	-0.0097 (7)	-0.0014 (7)	-0.0012 (7)
C4	0.0268 (9)	0.0325 (10)	0.0226 (8)	-0.0159 (8)	-0.0036 (7)	0.0044 (7)
C5	0.0328 (10)	0.0262 (10)	0.0292 (9)	-0.0154 (8)	-0.0113 (8)	0.0095 (7)
C6	0.0265 (9)	0.0177 (8)	0.0290 (9)	-0.0069 (7)	-0.0079 (7)	0.0025 (7)
C7	0.0202 (8)	0.0198 (8)	0.0205 (8)	-0.0074 (7)	-0.0045 (6)	0.0008 (6)
C8	0.0201 (8)	0.0133 (8)	0.0235 (8)	-0.0047 (6)	-0.0058 (6)	0.0002 (6)
C9	0.0198 (8)	0.0192 (8)	0.0221 (8)	-0.0072 (7)	-0.0037 (6)	-0.0007 (6)
C10	0.0278 (9)	0.0198 (9)	0.0285 (9)	-0.0040 (7)	-0.0009 (7)	-0.0012 (7)
C11	0.0274 (9)	0.0302 (10)	0.0283 (9)	-0.0060 (8)	0.0027 (7)	-0.0054 (8)
C12	0.0261 (8)	0.0323 (10)	0.0191 (8)	-0.0131 (8)	-0.0015 (7)	0.0015 (7)
C13	0.0345 (10)	0.0234 (9)	0.0283 (9)	-0.0114 (8)	-0.0029 (8)	0.0040 (7)
C14	0.0279 (9)	0.0197 (9)	0.0291 (9)	-0.0061 (7)	0.0024 (7)	-0.0010 (7)
C15	0.0215 (8)	0.0150 (8)	0.0283 (9)	-0.0054 (7)	-0.0053 (7)	-0.0012 (6)
C16	0.0215 (9)	0.0227 (9)	0.0403 (11)	-0.0065 (7)	-0.0011 (8)	-0.0057 (8)
C17	0.0263 (9)	0.0240 (10)	0.0699 (15)	-0.0047 (8)	-0.0149 (10)	-0.0091 (10)
C18	0.0558 (14)	0.0281 (11)	0.0552 (14)	-0.0124 (10)	-0.0337 (12)	-0.0003 (10)
C19	0.0761 (17)	0.0456 (14)	0.0295 (11)	-0.0333 (13)	-0.0178 (11)	0.0040 (10)
C20	0.0426 (12)	0.0387 (12)	0.0288 (10)	-0.0246 (10)	-0.0018 (9)	-0.0005 (8)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

Br—C12	1.8961 (18)	C9—C14	1.406 (2)
S—S <sup>i</sup>	3.2635 (8)	C10—C11	1.382 (3)
S—O2	1.4903 (13)	C10—H10	0.9300

S—C1	1.7721 (17)	C11—C12	1.378 (3)
S—C15	1.7996 (18)	C11—H11	0.9300
F—C4	1.365 (2)	C12—C13	1.379 (3)
O1—C7	1.375 (2)	C13—C14	1.380 (3)
O1—C8	1.3776 (19)	C13—H13	0.9300
C1—C8	1.374 (2)	C14—H14	0.9300
C1—C2	1.444 (2)	C15—C20	1.381 (3)
C2—C7	1.391 (2)	C15—C16	1.387 (2)
C2—C3	1.397 (2)	C16—C17	1.387 (3)
C3—C4	1.376 (3)	C16—H16	0.9300
C3—H3	0.9300	C17—C18	1.375 (4)
C4—C5	1.389 (3)	C17—H17	0.9300
C5—C6	1.384 (3)	C18—C19	1.388 (4)
C5—H5	0.9300	C18—H18	0.9300
C6—C7	1.382 (2)	C19—C20	1.390 (3)
C6—H6	0.9300	C19—H19	0.9300
C8—C9	1.455 (2)	C20—H20	0.9300
C9—C10	1.401 (2)		
O2—S—C1	107.56 (8)	C11—C10—H10	119.3
O2—S—C15	106.43 (8)	C9—C10—H10	119.3
C1—S—C15	96.72 (8)	C12—C11—C10	118.90 (18)
C7—O1—C8	106.98 (13)	C12—C11—H11	120.5
C8—C1—C2	107.73 (15)	C10—C11—H11	120.5
C8—C1—S	126.85 (13)	C11—C12—C13	121.57 (17)
C2—C1—S	125.42 (13)	C11—C12—Br	119.10 (14)
C7—C2—C3	119.78 (16)	C13—C12—Br	119.30 (14)
C7—C2—C1	104.55 (14)	C12—C13—C14	119.45 (18)
C3—C2—C1	135.66 (16)	C12—C13—H13	120.3
C4—C3—C2	115.72 (17)	C14—C13—H13	120.3
C4—C3—H3	122.1	C13—C14—C9	120.77 (18)
C2—C3—H3	122.1	C13—C14—H14	119.6
F—C4—C3	117.95 (18)	C9—C14—H14	119.6
F—C4—C5	117.67 (17)	C20—C15—C16	121.65 (18)
C3—C4—C5	124.38 (17)	C20—C15—S	118.49 (14)
C6—C5—C4	120.07 (17)	C16—C15—S	119.87 (15)
C6—C5—H5	120.0	C17—C16—C15	118.6 (2)
C4—C5—H5	120.0	C17—C16—H16	120.7
C7—C6—C5	116.00 (17)	C15—C16—H16	120.7
C7—C6—H6	122.0	C18—C17—C16	120.5 (2)
C5—C6—H6	122.0	C18—C17—H17	119.8
O1—C7—C6	124.94 (16)	C16—C17—H17	119.8
O1—C7—C2	111.03 (14)	C17—C18—C19	120.6 (2)
C6—C7—C2	124.03 (16)	C17—C18—H18	119.7
C1—C8—O1	109.69 (14)	C19—C18—H18	119.7
C1—C8—C9	135.70 (15)	C18—C19—C20	119.7 (2)
O1—C8—C9	114.61 (14)	C18—C19—H19	120.2
C10—C9—C14	117.93 (16)	C20—C19—H19	120.2
C10—C9—C8	119.97 (16)	C15—C20—C19	119.0 (2)
C14—C9—C8	122.10 (16)	C15—C20—H20	120.5

## supplementary materials

C11—C10—C9	121.35 (17)	C19—C20—H20	120.5
O2—S—C1—C8	-152.47 (14)	C7—O1—C8—C9	179.29 (13)
C15—S—C1—C8	97.90 (16)	C1—C8—C9—C10	-178.05 (18)
O2—S—C1—C2	28.34 (17)	O1—C8—C9—C10	1.2 (2)
C15—S—C1—C2	-81.29 (15)	C1—C8—C9—C14	2.0 (3)
C8—C1—C2—C7	-0.77 (18)	O1—C8—C9—C14	-178.71 (15)
S—C1—C2—C7	178.55 (12)	C14—C9—C10—C11	-0.5 (3)
C8—C1—C2—C3	178.37 (18)	C8—C9—C10—C11	179.57 (17)
S—C1—C2—C3	-2.3 (3)	C9—C10—C11—C12	-0.6 (3)
C7—C2—C3—C4	-0.9 (2)	C10—C11—C12—C13	1.5 (3)
C1—C2—C3—C4	-179.96 (18)	C10—C11—C12—Br	-176.61 (14)
C2—C3—C4—F	-179.75 (14)	C11—C12—C13—C14	-1.3 (3)
C2—C3—C4—C5	0.6 (3)	Br—C12—C13—C14	176.79 (15)
F—C4—C5—C6	-179.58 (15)	C12—C13—C14—C9	0.2 (3)
C3—C4—C5—C6	0.0 (3)	C10—C9—C14—C13	0.7 (3)
C4—C5—C6—C7	-0.4 (2)	C8—C9—C14—C13	-179.38 (17)
C8—O1—C7—C6	-179.14 (16)	O2—S—C15—C20	-13.32 (18)
C8—O1—C7—C2	0.74 (17)	C1—S—C15—C20	97.26 (17)
C5—C6—C7—O1	179.97 (15)	O2—S—C15—C16	166.15 (15)
C5—C6—C7—C2	0.1 (2)	C1—S—C15—C16	-83.27 (16)
C3—C2—C7—O1	-179.29 (14)	C20—C15—C16—C17	-2.5 (3)
C1—C2—C7—O1	0.02 (17)	S—C15—C16—C17	178.09 (15)
C3—C2—C7—C6	0.6 (2)	C15—C16—C17—C18	1.1 (3)
C1—C2—C7—C6	179.90 (16)	C16—C17—C18—C19	0.2 (3)
C2—C1—C8—O1	1.26 (18)	C17—C18—C19—C20	-0.3 (4)
S—C1—C8—O1	-178.05 (11)	C16—C15—C20—C19	2.4 (3)
C2—C1—C8—C9	-179.43 (17)	S—C15—C20—C19	-178.13 (17)
S—C1—C8—C9	1.3 (3)	C18—C19—C20—C15	-1.0 (4)
C7—O1—C8—C1	-1.24 (17)		

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

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

Cg3 is the centroid of the C15–C20 phenyl ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C5—H5 $\cdots$ Cg3 <sup>ii</sup>	0.93	2.85	3.644 (3)	145.

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



Fig. 1

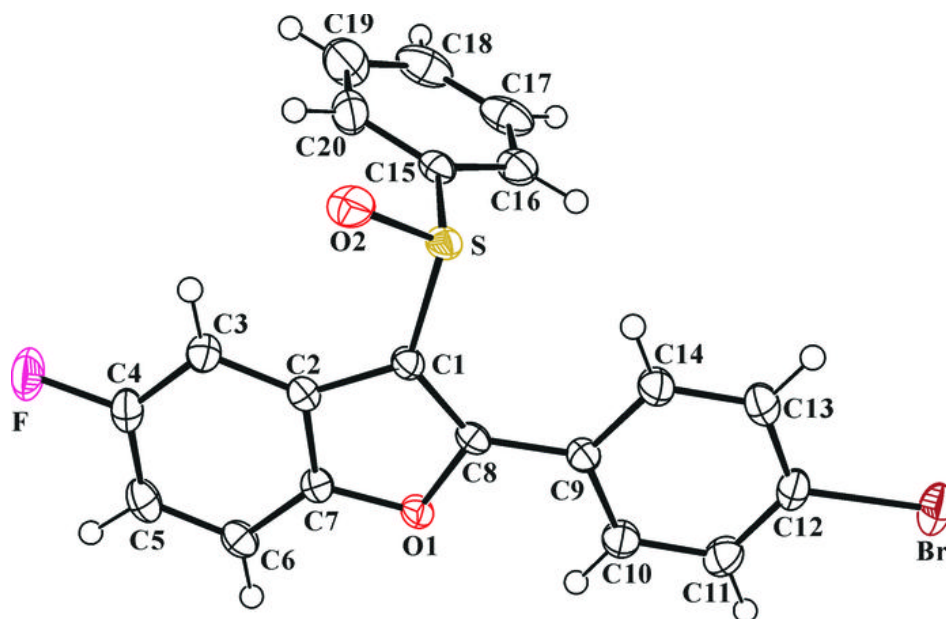


Fig. 2

