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3-(4-Fluorophenylsulfonyl)-5-isopropyl-2-methyl-1-benzofuran

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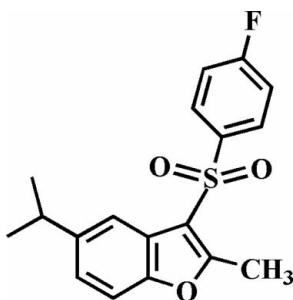
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Key indicators: single-crystal X-ray study; $T = 175$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.037; wR factor = 0.108; data-to-parameter ratio = 17.2.

In the title compound, $\text{C}_{18}\text{H}_{17}\text{FO}_3\text{S}$, the 4-fluorophenyl ring makes a dihedral angle of $82.12(4)^\circ$ with the plane of the benzofuran fragment. In the crystal structure, 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 crystal structures of similar 2-methyl-3-phenylsulfonyl-1-benzofuran derivatives, see: Choi *et al.* (2008*a,b*). For the biological 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).



Experimental

Crystal data

$\text{C}_{18}\text{H}_{17}\text{FO}_3\text{S}$
 $M_r = 332.38$
 Monoclinic, $P2_1/c$
 $a = 10.9434(6)$ Å
 $b = 11.3395(6)$ Å
 $c = 13.0988(7)$ Å
 $\beta = 100.252(3)^\circ$

$V = 1599.51(15)$ Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.23$ mm⁻¹
 $T = 175$ K
 $0.41 \times 0.29 \times 0.17$ mm

Data collection

Bruker SMART APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2009)
 $T_{\min} = 0.669$, $T_{\max} = 0.746$

14304 measured reflections
 3655 independent reflections
 3109 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.108$
 $S = 1.02$
 3655 reflections

212 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.36$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.37$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

Cg1 and Cg2 are the centroids of the C1/C2/C7/O3/C8 furan ring and the C2-C7 benzene ring, respectively.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C14}-\text{H14}\cdots\text{O2}^{\text{i}}$	0.95	2.51	3.401 (2)	155
$\text{C10}-\text{H10B}\cdots\text{Cg1}^{\text{ii}}$	0.98	2.86	3.561 (2)	120
$\text{C11}-\text{H11B}\cdots\text{Cg2}^{\text{ii}}$	0.98	2.91	3.670 (2)	135
$\text{C17}-\text{H17}\cdots\text{Cg2}^{\text{iii}}$	0.95	2.89	3.528 (2)	147

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

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: XU2750).

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supplementary materials

Acta Cryst. (2010). E66, o1067 [doi:10.1107/S1600536810012869]

3-(4-Fluorophenylsulfonyl)-5-isopropyl-2-methyl-1-benzofuran

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Comment

The compounds containing benzofuran ring show potent biological activities such as antifungal (Aslam *et al.*, 2006), antitumor and antiviral (Galal *et al.*, 2009), antimicrobial (Khan *et al.*, 2005) properties. These compounds occur widely in nature (Akgul & Anil, 2003; Soekamto *et al.*, 2003). As a part of our ongoing studies of the effect of side chain substituents on the solid state structures of 2-methyl-3-phenylsulfonyl-1-benzofuran analogues (Choi *et al.*, 2008*a,b*), we report the crystal structure of the title compound (Fig. 1).

The benzofuran unit is essentially planar, with a mean deviation of 0.113 (1) Å from the least-squares plane defined by the nine constituent atoms. The 4-fluorophenyl ring makes a dihedral angle of 82.12 (4)° with the plane of the benzofuran fragment. The molecular packing (Fig. 2) is stabilized by an intermolecular C—H...O hydrogen bond between the 4-fluorophenyl H atom and the oxygen of the sulfonyl group, with a C14—H14...O2ⁱ (Table 1). The crystal packing (Fig. 3) is further stabilized by three intermolecular C—H... π interactions; the first one between the methyl H atom of the isopropyl group and the furan ring of an adjacent molecule, with a C10—H10B...Cg1ⁱⁱ, the second one between the methyl H atom of the isopropyl group and the benzene ring of a neighbouring molecule, with a C11—H11B...Cg2ⁱⁱ, and the third one between the 4-fluorophenyl H atom and the benzene ring of an adjacent benzofuran system, with a C17—H17...Cg2ⁱⁱⁱ, respectively (Table 1; Cg1 and Cg2 are the centroids of the C1/C2/C7/O3/C8 furan ring and the C2–C7 benzene ring, respectively).

Experimental

77% 3-Chloroperoxybenzoic acid (448 mg, 2.0 mmol) was added in small portions to a stirred solution of 3-(4-fluorophenylsulfonyl)-5-isopropyl-2-methyl-1-benzofuran (270 mg, 0.9 mmol) in dichloromethane (40 mL) at 273 K. After being stirred at room temperature for 8 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 (silica gel, hexane–ethyl acetate, 2:1 v/v) to afford the title compound as a colorless solid [yield 79%, m.p. 402–403 K; R_f = 0.69 (hexane–ethyl acetate, 2:1 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 = 0.95 Å for aryl, 1.00 Å for methine and 0.98 Å for methyl H atoms, respectively. $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for aryl and methine, and $1.5U_{\text{eq}}(\text{C})$ for methyl H atoms.

Figures

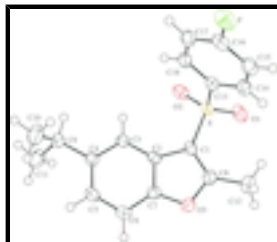


Fig. 1. The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are presented as a small spheres of arbitrary radius.

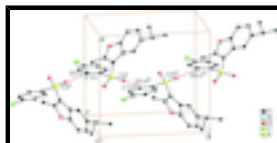


Fig. 2. C—H...O interactions (dotted lines) in the crystal structure of the title compound. [Symmetry codes: (i) $-x + 1, y - 1/2, -z + 1/2$; (iv) $-x + 1, y + 1/2, -z + 1/2$; (v) $x, y + 1, z$.]

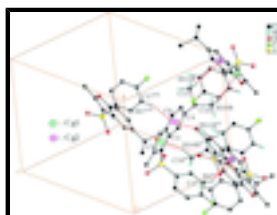


Fig. 3. C—H... π interactions (dotted lines) in the crystal structure of the title compound. Cg denotes the ring centroid. [Symmetry codes: (ii) $-x + 2, y + 1/2, -z + 1/2$; (iii) $x, -y + 1/2, z - 1/2$; (vi) $-x + 2, y - 1/2, -z + 1/2$; (vii) $x, -y + 1/2, z + 1/2$.]

3-(4-Fluorophenylsulfonyl)-5-isopropyl-2-methyl-1-benzofuran

Crystal data

$C_{18}H_{17}FO_3S$

$M_r = 332.38$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2ybc$

$a = 10.9434$ (6) Å

$b = 11.3395$ (6) Å

$c = 13.0988$ (7) Å

$\beta = 100.252$ (3)°

$V = 1599.51$ (15) Å³

$Z = 4$

$F(000) = 696$

$D_x = 1.380$ Mg m⁻³

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

Cell parameters from 6367 reflections

$\theta = 2.4$ – 27.5 °

$\mu = 0.23$ mm⁻¹

$T = 175$ K

Block, colourless

$0.41 \times 0.29 \times 0.17$ mm

Data collection

Bruker SMART APEXII CCD
diffractometer

Radiation source: rotating anode
graphite multilayer

Detector resolution: 10.0 pixels mm⁻¹

φ and ω scans

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

$T_{\min} = 0.669$, $T_{\max} = 0.746$

3655 independent reflections

3109 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.030$

$\theta_{\text{max}} = 27.5$ °, $\theta_{\text{min}} = 2.4$ °

$h = -14 \rightarrow 14$

$k = -14 \rightarrow 14$

$l = -16 \rightarrow 16$

14304 measured reflections

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.037$	H-atom parameters constrained
$wR(F^2) = 0.108$	$w = 1/[\sigma^2(F_o^2) + (0.0594P)^2 + 0.4509P]$
$S = 1.02$	where $P = (F_o^2 + 2F_c^2)/3$
3655 reflections	$(\Delta/\sigma)_{\max} < 0.001$
212 parameters	$\Delta\rho_{\max} = 0.36 \text{ e } \text{\AA}^{-3}$
0 restraints	$\Delta\rho_{\min} = -0.37 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: SHELXL97 (Sheldrick, 2008), $F_c^* = kF_c[1+0.001xF_c^2\lambda^3/\sin(2\theta)]^{-1/4}$
	Extinction coefficient: 0.0117 (15)

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>	$U_{\text{iso}}^*/U_{\text{eq}}$
S	0.54221 (3)	0.13196 (3)	0.21925 (3)	0.02922 (13)
F	0.75485 (9)	-0.21439 (9)	-0.02852 (8)	0.0475 (3)
O1	0.44396 (10)	0.07695 (11)	0.26153 (9)	0.0415 (3)
O2	0.51752 (10)	0.23800 (9)	0.15885 (8)	0.0367 (3)
O3	0.79447 (10)	0.15165 (9)	0.47328 (8)	0.0300 (2)
C1	0.66335 (13)	0.16383 (12)	0.32124 (11)	0.0268 (3)
C2	0.75540 (12)	0.25570 (12)	0.32202 (10)	0.0244 (3)
C3	0.78117 (13)	0.34256 (12)	0.25361 (11)	0.0270 (3)
H3	0.7288	0.3527	0.1881	0.032*
C4	0.88480 (13)	0.41423 (13)	0.28261 (11)	0.0285 (3)
C5	0.96004 (13)	0.39900 (13)	0.38020 (11)	0.0302 (3)
H5	1.0300	0.4491	0.3993	0.036*
C6	0.93628 (13)	0.31367 (13)	0.44994 (11)	0.0297 (3)
H6	0.9877	0.3038	0.5159	0.036*
C7	0.83340 (13)	0.24398 (12)	0.41752 (10)	0.0257 (3)
C8	0.69246 (14)	0.10323 (13)	0.41204 (11)	0.0303 (3)

supplementary materials

C9	0.91774 (15)	0.50549 (14)	0.20723 (12)	0.0356 (4)
H9	0.8483	0.5073	0.1462	0.043*
C10	1.0351 (2)	0.47032 (18)	0.16761 (16)	0.0548 (5)
H10A	1.1061	0.4728	0.2249	0.082*
H10B	1.0492	0.5253	0.1132	0.082*
H10C	1.0256	0.3902	0.1392	0.082*
C11	0.9299 (2)	0.62926 (15)	0.25374 (16)	0.0531 (5)
H11A	0.8558	0.6477	0.2832	0.080*
H11B	0.9381	0.6866	0.1994	0.080*
H11C	1.0036	0.6329	0.3085	0.080*
C12	0.64435 (18)	-0.00464 (15)	0.45463 (14)	0.0452 (4)
H12A	0.5675	-0.0294	0.4094	0.068*
H12B	0.6275	0.0117	0.5243	0.068*
H12C	0.7062	-0.0677	0.4584	0.068*
C13	0.60386 (13)	0.02725 (12)	0.14291 (11)	0.0274 (3)
C14	0.60321 (15)	-0.09153 (13)	0.16991 (12)	0.0342 (3)
H14	0.5684	-0.1159	0.2279	0.041*
C15	0.65382 (15)	-0.17364 (14)	0.11133 (13)	0.0375 (4)
H15	0.6546	-0.2551	0.1283	0.045*
C16	0.70315 (14)	-0.13427 (13)	0.02763 (13)	0.0332 (3)
C17	0.70304 (14)	-0.01834 (14)	-0.00155 (12)	0.0344 (3)
H17	0.7364	0.0049	-0.0606	0.041*
C18	0.65300 (14)	0.06423 (13)	0.05734 (12)	0.0309 (3)
H18	0.6523	0.1454	0.0394	0.037*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S	0.0237 (2)	0.0283 (2)	0.0349 (2)	-0.00195 (13)	0.00319 (14)	-0.00717 (14)
F	0.0421 (6)	0.0428 (6)	0.0595 (7)	0.0017 (4)	0.0145 (5)	-0.0195 (5)
O1	0.0295 (6)	0.0473 (7)	0.0503 (7)	-0.0098 (5)	0.0138 (5)	-0.0133 (5)
O2	0.0336 (6)	0.0308 (6)	0.0412 (6)	0.0052 (4)	-0.0057 (5)	-0.0056 (5)
O3	0.0344 (6)	0.0300 (5)	0.0254 (5)	-0.0011 (4)	0.0047 (4)	0.0015 (4)
C1	0.0263 (7)	0.0248 (7)	0.0296 (7)	-0.0011 (5)	0.0061 (5)	-0.0042 (5)
C2	0.0238 (6)	0.0237 (7)	0.0254 (7)	0.0010 (5)	0.0033 (5)	-0.0044 (5)
C3	0.0282 (7)	0.0272 (7)	0.0238 (7)	-0.0006 (5)	0.0001 (5)	-0.0015 (5)
C4	0.0309 (7)	0.0270 (7)	0.0280 (7)	-0.0026 (6)	0.0060 (6)	-0.0031 (6)
C5	0.0276 (7)	0.0305 (7)	0.0317 (8)	-0.0043 (6)	0.0032 (6)	-0.0058 (6)
C6	0.0299 (7)	0.0317 (7)	0.0253 (7)	0.0021 (6)	-0.0009 (5)	-0.0044 (6)
C7	0.0296 (7)	0.0248 (7)	0.0229 (7)	0.0026 (5)	0.0055 (5)	-0.0014 (5)
C8	0.0318 (7)	0.0298 (7)	0.0307 (8)	-0.0016 (6)	0.0096 (6)	-0.0033 (6)
C9	0.0429 (9)	0.0341 (8)	0.0288 (7)	-0.0112 (7)	0.0035 (6)	0.0009 (6)
C10	0.0683 (13)	0.0476 (11)	0.0569 (12)	-0.0131 (9)	0.0341 (10)	-0.0023 (9)
C11	0.0834 (14)	0.0304 (9)	0.0503 (11)	-0.0054 (9)	0.0247 (10)	0.0037 (8)
C12	0.0516 (10)	0.0413 (9)	0.0444 (10)	-0.0111 (8)	0.0130 (8)	0.0077 (8)
C13	0.0245 (7)	0.0263 (7)	0.0302 (7)	-0.0030 (5)	0.0023 (5)	-0.0041 (6)
C14	0.0398 (8)	0.0281 (7)	0.0351 (8)	-0.0050 (6)	0.0080 (6)	-0.0006 (6)
C15	0.0423 (9)	0.0249 (7)	0.0445 (9)	-0.0006 (6)	0.0054 (7)	-0.0022 (7)

C16	0.0248 (7)	0.0340 (8)	0.0396 (9)	-0.0004 (6)	0.0029 (6)	-0.0126 (6)
C17	0.0315 (8)	0.0378 (8)	0.0349 (8)	-0.0083 (6)	0.0087 (6)	-0.0040 (6)
C18	0.0303 (7)	0.0269 (7)	0.0350 (8)	-0.0057 (6)	0.0046 (6)	-0.0004 (6)

Geometric parameters (Å, °)

S—O1	1.437 (1)	C9—C11	1.526 (2)
S—O2	1.438 (1)	C9—H9	1.0000
S—C1	1.744 (2)	C10—H10A	0.9800
S—C13	1.762 (1)	C10—H10B	0.9800
F—C16	1.355 (2)	C10—H10C	0.9800
O3—C8	1.368 (2)	C11—H11A	0.9800
O3—C7	1.386 (2)	C11—H11B	0.9800
C1—C8	1.361 (2)	C11—H11C	0.9800
C1—C2	1.448 (2)	C12—H12A	0.9800
C2—C7	1.390 (2)	C12—H12B	0.9800
C2—C3	1.394 (2)	C12—H12C	0.9800
C3—C4	1.392 (2)	C13—C14	1.393 (2)
C3—H3	0.9500	C13—C18	1.391 (2)
C4—C5	1.403 (2)	C14—C15	1.383 (2)
C4—C9	1.517 (2)	C14—H14	0.9500
C5—C6	1.387 (2)	C15—C16	1.380 (2)
C5—H5	0.9500	C15—H15	0.9500
C6—C7	1.379 (2)	C16—C17	1.369 (2)
C6—H6	0.9500	C17—C18	1.386 (2)
C8—C12	1.480 (2)	C17—H17	0.9500
C9—C10	1.521 (2)	C18—H18	0.9500
O1—S—O2	119.66 (7)	C9—C10—H10A	109.5
O1—S—C1	108.28 (7)	C9—C10—H10B	109.5
O2—S—C1	106.91 (7)	H10A—C10—H10B	109.5
O1—S—C13	108.33 (7)	C9—C10—H10C	109.5
O2—S—C13	107.74 (7)	H10A—C10—H10C	109.5
C1—S—C13	104.99 (7)	H10B—C10—H10C	109.5
C8—O3—C7	106.82 (11)	C9—C11—H11A	109.5
C8—C1—C2	107.62 (13)	C9—C11—H11B	109.5
C8—C1—S	126.33 (11)	H11A—C11—H11B	109.5
C2—C1—S	125.97 (11)	C9—C11—H11C	109.5
C7—C2—C3	118.96 (12)	H11A—C11—H11C	109.5
C7—C2—C1	104.63 (12)	H11B—C11—H11C	109.5
C3—C2—C1	136.39 (13)	C8—C12—H12A	109.5
C4—C3—C2	119.04 (13)	C8—C12—H12B	109.5
C4—C3—H3	120.5	H12A—C12—H12B	109.5
C2—C3—H3	120.5	C8—C12—H12C	109.5
C3—C4—C5	119.64 (13)	H12A—C12—H12C	109.5
C3—C4—C9	119.80 (13)	H12B—C12—H12C	109.5
C5—C4—C9	120.53 (13)	C14—C13—C18	121.08 (14)
C6—C5—C4	122.53 (13)	C14—C13—S	119.19 (11)
C6—C5—H5	118.7	C18—C13—S	119.73 (11)
C4—C5—H5	118.7	C15—C14—C13	119.29 (14)

supplementary materials

C7—C6—C5	115.82 (13)	C15—C14—H14	120.4
C7—C6—H6	122.1	C13—C14—H14	120.4
C5—C6—H6	122.1	C16—C15—C14	118.36 (14)
C6—C7—O3	125.53 (13)	C16—C15—H15	120.8
C6—C7—C2	124.01 (13)	C14—C15—H15	120.8
O3—C7—C2	110.45 (12)	F—C16—C17	118.17 (14)
C1—C8—O3	110.44 (13)	F—C16—C15	118.35 (14)
C1—C8—C12	134.67 (15)	C17—C16—C15	123.48 (14)
O3—C8—C12	114.75 (13)	C16—C17—C18	118.29 (14)
C4—C9—C10	110.85 (14)	C16—C17—H17	120.9
C4—C9—C11	112.42 (13)	C18—C17—H17	120.9
C10—C9—C11	110.99 (15)	C17—C18—C13	119.49 (14)
C4—C9—H9	107.4	C17—C18—H18	120.3
C10—C9—H9	107.4	C13—C18—H18	120.3
C11—C9—H9	107.4		

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C14—H14 \cdots O2 ⁱ	0.95	2.51	3.401 (2)	155.
C10—H10B \cdots Cg1 ⁱⁱ	0.98	2.86	3.561 (2)	120.
C11—H11B \cdots Cg2 ⁱⁱ	0.98	2.91	3.670 (2)	135.
C17—H17 \cdots Cg2 ⁱⁱⁱ	0.95	2.89	3.528 (2)	147.

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

Fig. 1

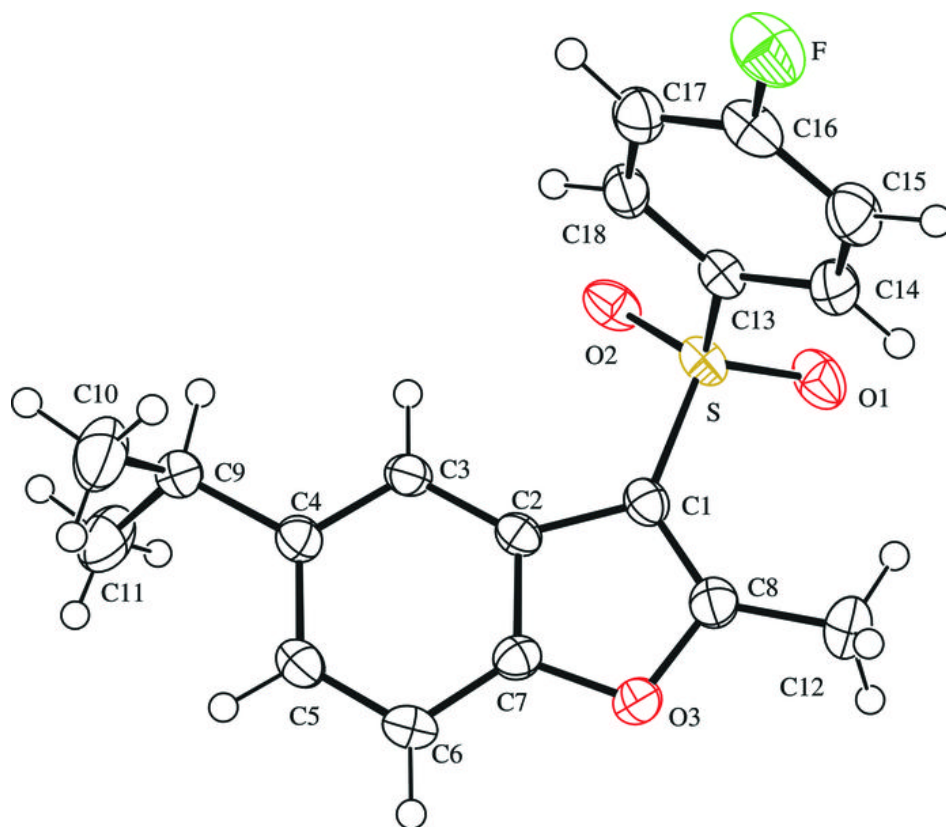


Fig. 2

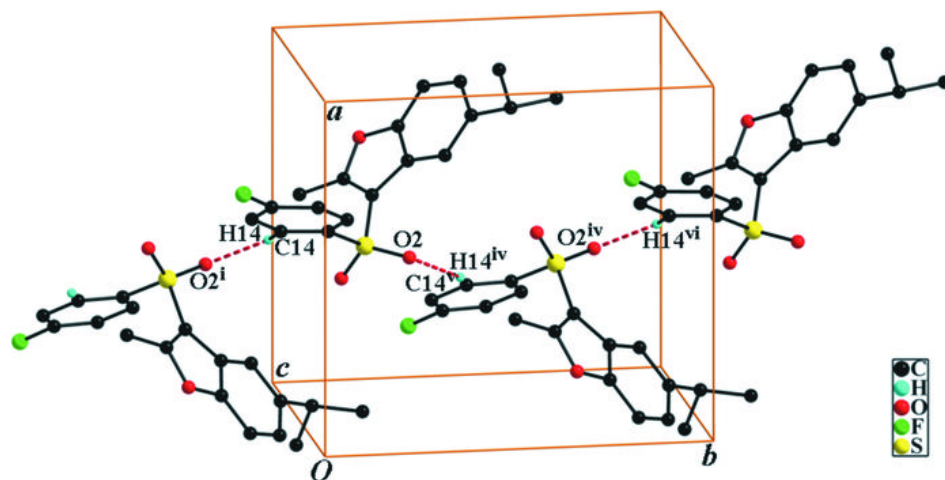


Fig. 3

