

2,5-Bis(4-fluorophenyl)-2-methylsulfanyl-1-benzofuran

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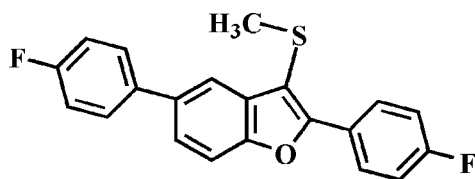
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Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.038; wR factor = 0.101; data-to-parameter ratio = 16.3.

The crystal studied of the title compound, $\text{C}_{21}\text{H}_{14}\text{F}_2\text{OS}$, was an inversion twin with a 0.67 (8):0.33 (8) domain ratio. The 4-fluorophenyl ring in the 2-position makes a dihedral angle of 25.14 (6°) with the mean plane of the benzofuran fragment, and the dihedral angle between 4-fluorophenyl ring in the 5-position and the mean plane of the benzofuran fragment is 28.50 (7°). In the crystal, molecules are linked through weak intermolecular $\text{C}-\text{H}\cdots\text{F}$ and $\text{C}-\text{H}\cdots\pi$ interactions.

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 structural studies of related 3-alkylsulfanyl-2-(4-fluorophenyl)-5-phenyl-1-benzofuran derivatives, see: Choi *et al.* (2009, 2010).



Experimental

Crystal data

$\text{C}_{21}\text{H}_{14}\text{F}_2\text{OS}$
 $M_r = 352.38$
 Monoclinic, $P2_1$

$a = 10.7673$ (7) Å
 $b = 7.2986$ (5) Å
 $c = 11.5145$ (8) Å

$\beta = 116.124$ (1°)
 $V = 812.44$ (10) Å³
 $Z = 2$
 Mo $K\alpha$ radiation

$\mu = 0.23$ mm⁻¹
 $T = 173$ K
 $0.32 \times 0.29 \times 0.13$ mm

Data collection

Bruker SMART APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2009)
 $T_{\min} = 0.930$, $T_{\max} = 0.972$

7891 measured reflections
 3710 independent reflections
 3501 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.101$
 $S = 1.06$
 3710 reflections
 228 parameters
 1 restraint

H-atom parameters constrained
 $\Delta\rho_{\max} = 0.33$ e Å⁻³
 $\Delta\rho_{\min} = -0.21$ e Å⁻³
 Absolute structure: Flack (1983),
 1700 Friedel pairs
 Flack parameter: 0.33 (8)

Table 1

Hydrogen-bond geometry (Å, °).

C_g is the centroid of the C15–C20 4-fluorophenyl ring.

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---------------------------|-------|-------------|-------------|---------------|
| $C6-H6\cdots F1^i$ | 0.95 | 2.45 | 3.322 (2) | 153 |
| $C10-H10\cdots C_g^{ii}$ | 0.95 | 2.67 | 3.441 (2) | 139 |
| $C17-H17\cdots C_g^{iii}$ | 0.95 | 2.86 | 3.557 (2) | 131 |

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

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: SJ5110).

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supplementary materials

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2,5-Bis(4-fluorophenyl)-2-methylsulfanyl-1-benzofuran

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Comment

Many compounds having a benzofuran ring system exhibit interesting pharmacological properties such as antifungal, anti-tumor and antiviral, and antimicrobial activities (Aslam *et al.*, 2006, Galal *et al.*, 2009, Khan *et al.*, 2005). These compounds occur in a wide range of natural products (Akgul & Anil, 2003; Soekamto *et al.*, 2003). As a part of our ongoing study of substituent effects on the solid state structures of 3-alkylsulfanyl-2-(4-fluorophenyl)-5-phenyl-1-benzofuran analogues (Choi *et al.*, 2009, 2010), we report herein on the crystal structure of the title compound.

The title compound crystallizes as the non-centrosymmetric space group $P2_1$ in spite of having no asymmetric C atoms. The crystal studied was an inversion twin with a 0.33 (8) : 0.67 (8) domain ratio.

In the title molecule (Fig. 1), the benzofuran unit is essentially planar, with a mean deviation of 0.009 (1) Å from the least-squares plane defined by the nine constituent atoms. In the crystal structure, the dihedral angle formed by the 4-fluorophenyl ring (C15–C20) and the mean plane of the benzofuran fragment is 25.14 (6)°, and the (C9–C14) 4-fluorophenyl ring makes a dihedral angle of 28.50 (7)° with the mean plane of the benzofuran fragment. The molecular packing (Fig. 2) is stabilized by weak intermolecular C—H...F hydrogen bonds between a benzene H atom and the F atom of the (C9–C14) 4-fluorophenyl ring (Table 1; C6—H6...F1ⁱ). The molecular packing (Fig. 3) also exhibits intermolecular C—H... π interactions; the first one between a 4-fluorophenyl H atom in the 5-position and the (C15–C20) 4-fluorophenyl ring (Table 1; C10—H10...Cgⁱⁱ), and the second one between the 4-fluorophenyl H atom in the 2-position and the (C15–C20) 4-fluorophenyl ring (Table 1; C17—H17...Cgⁱⁱⁱ) (Cg is the centroid of the C15–C20 4-fluorophenyl ring).

Experimental

Zinc chloride (245 mg, 1.8 mmol) was added to a stirred solution of 4-fluoro-4'-hydroxybiphenyl (339 mg, 1.8 mmol) and 2-chloro-4'-fluoro-2-methylsulfanylacetophenone (395 mg, 1.8 mmol) in dichloromethane (30 mL) at room temperature, and stirring was continued at the same temperature for 40 min. The reaction was quenched by the addition of water and the organic layer was separated, dried over magnesium sulfate, filtered and concentrated at reduced pressure. The residue was purified by column chromatography (carbon tetrachloride) to afford the title compound as a colorless solid [yield 65%, m.p. 438–439 K; R_f = 0.69 (carbon tetrachloride)]. 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

The reported Flack parameter was obtained by TWIN/BASF procedure in SHELXL (Sheldrick, 2008). 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.

Figures

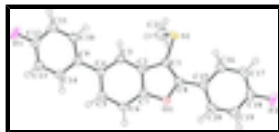


Fig. 1. The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are presented as a small spheres of arbitrary radius.

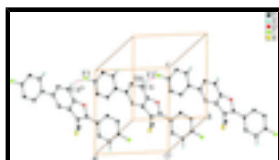


Fig. 2. A view of the C—H...F interactions (dotted lines) in the crystal structure of the title compound. [Symmetry codes: (i) $x - 1, y, z$; (iv) $x + 1, y, z$.]

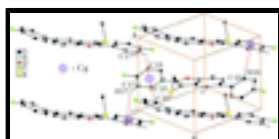


Fig. 3. A view of the C—H... π interactions (dotted lines) in the crystal structure of the title compound. [Symmetry codes: (ii) $-x + 1, y + 1/2, -z + 1$; (iii) $-x, y - 1/2, -z$; (v) $1 - x, y - 1/2, -z + 1$; (vi) $-x, y + 1/2, -z$.]

2,5-Bis(4-fluorophenyl)-2-methylsulfanyl-1-benzofuran

Crystal data

| | |
|---------------------------------|---|
| $C_{21}H_{14}F_2OS$ | $F(000) = 364$ |
| $M_r = 352.38$ | $D_x = 1.440 \text{ Mg m}^{-3}$ |
| Monoclinic, $P2_1$ | Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$ |
| Hall symbol: P 2yb | Cell parameters from 3532 reflections |
| $a = 10.7673 (7) \text{ \AA}$ | $\theta = 2.2\text{--}27.1^\circ$ |
| $b = 7.2986 (5) \text{ \AA}$ | $\mu = 0.23 \text{ mm}^{-1}$ |
| $c = 11.5145 (8) \text{ \AA}$ | $T = 173 \text{ K}$ |
| $\beta = 116.124 (1)^\circ$ | Block, colourless |
| $V = 812.44 (10) \text{ \AA}^3$ | $0.32 \times 0.29 \times 0.13 \text{ mm}$ |
| $Z = 2$ | |

Data collection

| | |
|--|---|
| Bruker SMART APEXII CCD diffractometer | 3710 independent reflections |
| Radiation source: rotating anode graphite multilayer | 3501 reflections with $I > 2\sigma(I)$ |
| Detector resolution: $10.0 \text{ pixels mm}^{-1}$ | $R_{\text{int}} = 0.023$ |
| φ and ω scans | $\theta_{\text{max}} = 27.5^\circ, \theta_{\text{min}} = 2.0^\circ$ |
| Absorption correction: multi-scan (SADABS; Bruker, 2009) | $h = -13 \rightarrow 13$ |
| $T_{\text{min}} = 0.930, T_{\text{max}} = 0.972$ | $k = -9 \rightarrow 9$ |
| 7891 measured reflections | $l = -14 \rightarrow 14$ |

Refinement

| | |
|---------------------|--|
| Refinement on F^2 | Secondary atom site location: difference Fourier map |
|---------------------|--|

| | |
|--|--|
| Least-squares matrix: full | Hydrogen site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.038$ | H-atom parameters constrained |
| $wR(F^2) = 0.101$ | $w = 1/[\sigma^2(F_o^2) + (0.056P)^2 + 0.1486P]$ |
| $S = 1.06$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 3710 reflections | $(\Delta/\sigma)_{\max} < 0.001$ |
| 228 parameters | $\Delta\rho_{\max} = 0.33 \text{ e } \text{\AA}^{-3}$ |
| 1 restraint | $\Delta\rho_{\min} = -0.21 \text{ e } \text{\AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Absolute structure: Flack (1983), 1700 Friedel pairs |
| | Flack parameter: 0.33 (8) |

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)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|---------------|-------------|---------------|----------------------------------|
| S1 | 0.43705 (5) | 0.35582 (9) | 0.12177 (4) | 0.03705 (15) |
| F1 | 1.36155 (13) | 0.4416 (2) | 0.73988 (15) | 0.0491 (4) |
| F2 | -0.24680 (12) | 0.4131 (2) | -0.00514 (13) | 0.0463 (3) |
| O1 | 0.36309 (13) | 0.4157 (2) | 0.42787 (12) | 0.0294 (3) |
| C1 | 0.43510 (19) | 0.3862 (3) | 0.27194 (17) | 0.0269 (4) |
| C2 | 0.55585 (18) | 0.3959 (3) | 0.39519 (16) | 0.0253 (4) |
| C3 | 0.69845 (18) | 0.3930 (3) | 0.43512 (17) | 0.0260 (4) |
| H3 | 0.7346 | 0.3790 | 0.3738 | 0.031* |
| C4 | 0.78673 (18) | 0.4111 (3) | 0.56623 (17) | 0.0243 (4) |
| C5 | 0.7295 (2) | 0.4268 (3) | 0.65587 (18) | 0.0280 (4) |
| H5 | 0.7905 | 0.4363 | 0.7454 | 0.034* |
| C6 | 0.5895 (2) | 0.4287 (3) | 0.61797 (18) | 0.0303 (4) |
| H6 | 0.5523 | 0.4395 | 0.6788 | 0.036* |
| C7 | 0.5052 (2) | 0.4142 (3) | 0.48647 (18) | 0.0277 (4) |
| C8 | 0.32360 (19) | 0.3989 (3) | 0.29668 (17) | 0.0273 (4) |
| C9 | 0.93978 (18) | 0.4152 (3) | 0.61213 (16) | 0.0243 (4) |
| C10 | 1.0238 (2) | 0.5099 (3) | 0.72483 (19) | 0.0290 (4) |
| H10 | 0.9826 | 0.5693 | 0.7726 | 0.035* |
| C11 | 1.1652 (2) | 0.5193 (3) | 0.7686 (2) | 0.0344 (5) |
| H11 | 1.2214 | 0.5846 | 0.8453 | 0.041* |
| C12 | 1.2229 (2) | 0.4318 (3) | 0.6983 (2) | 0.0320 (4) |
| C13 | 1.1449 (2) | 0.3356 (3) | 0.58707 (19) | 0.0334 (4) |

supplementary materials

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|------|--------------|------------|--------------|------------|
| H13 | 1.1873 | 0.2764 | 0.5402 | 0.040* |
| C14 | 1.0033 (2) | 0.3270 (3) | 0.54499 (19) | 0.0297 (4) |
| H14 | 0.9482 | 0.2598 | 0.4689 | 0.036* |
| C15 | 0.17419 (19) | 0.4016 (3) | 0.21639 (17) | 0.0261 (4) |
| C16 | 0.1142 (2) | 0.3192 (3) | 0.09396 (18) | 0.0298 (4) |
| H16 | 0.1714 | 0.2610 | 0.0615 | 0.036* |
| C17 | -0.0278 (2) | 0.3218 (3) | 0.01996 (18) | 0.0315 (4) |
| H17 | -0.0688 | 0.2643 | -0.0624 | 0.038* |
| C18 | -0.1079 (2) | 0.4093 (3) | 0.06815 (19) | 0.0313 (4) |
| C19 | -0.0530 (2) | 0.4919 (3) | 0.1888 (2) | 0.0328 (4) |
| H19 | -0.1112 | 0.5506 | 0.2200 | 0.039* |
| C20 | 0.0880 (2) | 0.4865 (3) | 0.26212 (19) | 0.0293 (4) |
| H20 | 0.1275 | 0.5415 | 0.3454 | 0.035* |
| C21 | 0.5127 (3) | 0.5682 (4) | 0.1057 (3) | 0.0520 (7) |
| H21A | 0.4539 | 0.6705 | 0.1061 | 0.078* |
| H21B | 0.5206 | 0.5683 | 0.0241 | 0.078* |
| H21C | 0.6048 | 0.5817 | 0.1781 | 0.078* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|-------------|-------------|
| S1 | 0.0418 (3) | 0.0475 (3) | 0.0259 (2) | -0.0051 (2) | 0.0186 (2) | -0.0059 (2) |
| F1 | 0.0243 (6) | 0.0571 (9) | 0.0646 (9) | 0.0009 (6) | 0.0185 (6) | -0.0050 (7) |
| F2 | 0.0245 (6) | 0.0532 (9) | 0.0509 (7) | 0.0006 (6) | 0.0073 (5) | 0.0010 (6) |
| O1 | 0.0258 (6) | 0.0405 (8) | 0.0231 (6) | -0.0011 (6) | 0.0119 (5) | -0.0019 (6) |
| C1 | 0.0279 (9) | 0.0307 (10) | 0.0228 (8) | -0.0028 (8) | 0.0118 (7) | -0.0028 (7) |
| C2 | 0.0295 (9) | 0.0258 (10) | 0.0219 (8) | -0.0014 (7) | 0.0125 (7) | -0.0011 (7) |
| C3 | 0.0281 (9) | 0.0286 (10) | 0.0256 (8) | -0.0024 (8) | 0.0157 (7) | -0.0011 (8) |
| C4 | 0.0269 (9) | 0.0207 (8) | 0.0265 (8) | 0.0014 (7) | 0.0128 (7) | 0.0010 (7) |
| C5 | 0.0266 (9) | 0.0317 (10) | 0.0228 (8) | 0.0013 (8) | 0.0083 (7) | 0.0001 (8) |
| C6 | 0.0327 (10) | 0.0372 (11) | 0.0253 (9) | 0.0010 (8) | 0.0165 (8) | -0.0004 (8) |
| C7 | 0.0249 (8) | 0.0317 (10) | 0.0275 (9) | -0.0012 (8) | 0.0124 (7) | -0.0004 (8) |
| C8 | 0.0303 (9) | 0.0282 (10) | 0.0233 (8) | -0.0024 (8) | 0.0116 (7) | -0.0004 (7) |
| C9 | 0.0250 (9) | 0.0217 (8) | 0.0259 (8) | 0.0020 (7) | 0.0109 (7) | 0.0054 (7) |
| C10 | 0.0286 (10) | 0.0316 (10) | 0.0290 (9) | 0.0029 (8) | 0.0146 (8) | -0.0024 (8) |
| C11 | 0.0298 (10) | 0.0362 (11) | 0.0321 (10) | 0.0004 (9) | 0.0091 (8) | -0.0049 (9) |
| C12 | 0.0240 (9) | 0.0319 (10) | 0.0417 (11) | 0.0032 (8) | 0.0159 (8) | 0.0035 (9) |
| C13 | 0.0366 (10) | 0.0317 (10) | 0.0397 (10) | 0.0057 (9) | 0.0240 (9) | -0.0010 (9) |
| C14 | 0.0326 (10) | 0.0265 (10) | 0.0309 (9) | 0.0016 (8) | 0.0147 (8) | -0.0019 (8) |
| C15 | 0.0268 (9) | 0.0246 (9) | 0.0263 (8) | -0.0022 (8) | 0.0112 (7) | 0.0016 (7) |
| C16 | 0.0318 (10) | 0.0287 (10) | 0.0285 (9) | -0.0017 (8) | 0.0128 (8) | -0.0009 (8) |
| C17 | 0.0346 (11) | 0.0302 (11) | 0.0238 (9) | -0.0029 (8) | 0.0075 (8) | -0.0007 (8) |
| C18 | 0.0249 (9) | 0.0289 (10) | 0.0337 (9) | -0.0012 (8) | 0.0071 (8) | 0.0059 (8) |
| C19 | 0.0316 (11) | 0.0305 (10) | 0.0397 (11) | 0.0022 (8) | 0.0188 (9) | 0.0003 (9) |
| C20 | 0.0341 (11) | 0.0259 (9) | 0.0262 (9) | -0.0020 (8) | 0.0117 (8) | -0.0017 (7) |
| C21 | 0.0554 (16) | 0.0591 (17) | 0.0478 (14) | -0.0053 (12) | 0.0286 (13) | 0.0144 (12) |

Geometric parameters (Å, °)

| | | | |
|-----------|-------------|-------------|-------------|
| S1—C1 | 1.7527 (18) | C10—C11 | 1.379 (3) |
| S1—C21 | 1.798 (3) | C10—H10 | 0.9500 |
| F1—C12 | 1.354 (2) | C11—C12 | 1.375 (3) |
| F2—C18 | 1.355 (2) | C11—H11 | 0.9500 |
| O1—C7 | 1.374 (2) | C12—C13 | 1.375 (3) |
| O1—C8 | 1.383 (2) | C13—C14 | 1.384 (3) |
| C1—C8 | 1.354 (3) | C13—H13 | 0.9500 |
| C1—C2 | 1.444 (2) | C14—H14 | 0.9500 |
| C2—C7 | 1.387 (2) | C15—C20 | 1.398 (3) |
| C2—C3 | 1.396 (2) | C15—C16 | 1.402 (3) |
| C3—C4 | 1.392 (2) | C16—C17 | 1.384 (3) |
| C3—H3 | 0.9500 | C16—H16 | 0.9500 |
| C4—C5 | 1.420 (3) | C17—C18 | 1.372 (3) |
| C4—C9 | 1.493 (2) | C17—H17 | 0.9500 |
| C5—C6 | 1.373 (3) | C18—C19 | 1.385 (3) |
| C5—H5 | 0.9500 | C19—C20 | 1.375 (3) |
| C6—C7 | 1.385 (3) | C19—H19 | 0.9500 |
| C6—H6 | 0.9500 | C20—H20 | 0.9500 |
| C8—C15 | 1.461 (3) | C21—H21A | 0.9800 |
| C9—C14 | 1.395 (3) | C21—H21B | 0.9800 |
| C9—C10 | 1.395 (3) | C21—H21C | 0.9800 |
| C1—S1—C21 | 101.24 (12) | C10—C11—H11 | 120.9 |
| C7—O1—C8 | 106.02 (14) | F1—C12—C13 | 118.83 (18) |
| C8—C1—C2 | 106.74 (15) | F1—C12—C11 | 118.70 (19) |
| C8—C1—S1 | 127.83 (14) | C13—C12—C11 | 122.47 (18) |
| C2—C1—S1 | 125.39 (14) | C12—C13—C14 | 118.42 (18) |
| C7—C2—C3 | 119.62 (16) | C12—C13—H13 | 120.8 |
| C7—C2—C1 | 105.38 (15) | C14—C13—H13 | 120.8 |
| C3—C2—C1 | 134.99 (16) | C13—C14—C9 | 121.27 (18) |
| C4—C3—C2 | 118.87 (16) | C13—C14—H14 | 119.4 |
| C4—C3—H3 | 120.6 | C9—C14—H14 | 119.4 |
| C2—C3—H3 | 120.6 | C20—C15—C16 | 118.72 (17) |
| C3—C4—C5 | 119.24 (17) | C20—C15—C8 | 119.79 (17) |
| C3—C4—C9 | 120.40 (16) | C16—C15—C8 | 121.49 (17) |
| C5—C4—C9 | 120.36 (16) | C17—C16—C15 | 120.55 (18) |
| C6—C5—C4 | 122.47 (17) | C17—C16—H16 | 119.7 |
| C6—C5—H5 | 118.8 | C15—C16—H16 | 119.7 |
| C4—C5—H5 | 118.8 | C18—C17—C16 | 118.58 (18) |
| C5—C6—C7 | 116.47 (17) | C18—C17—H17 | 120.7 |
| C5—C6—H6 | 121.8 | C16—C17—H17 | 120.7 |
| C7—C6—H6 | 121.8 | F2—C18—C17 | 118.40 (18) |
| O1—C7—C6 | 126.02 (17) | F2—C18—C19 | 118.85 (19) |
| O1—C7—C2 | 110.67 (15) | C17—C18—C19 | 122.75 (18) |
| C6—C7—C2 | 123.31 (17) | C20—C19—C18 | 118.17 (19) |
| C1—C8—O1 | 111.18 (15) | C20—C19—H19 | 120.9 |
| C1—C8—C15 | 134.39 (17) | C18—C19—H19 | 120.9 |

supplementary materials

| | | | |
|--------------|--------------|-----------------|--------------|
| O1—C8—C15 | 114.42 (15) | C19—C20—C15 | 121.21 (18) |
| C14—C9—C10 | 117.96 (17) | C19—C20—H20 | 119.4 |
| C14—C9—C4 | 121.93 (16) | C15—C20—H20 | 119.4 |
| C10—C9—C4 | 120.11 (16) | S1—C21—H21A | 109.5 |
| C11—C10—C9 | 121.60 (18) | S1—C21—H21B | 109.5 |
| C11—C10—H10 | 119.2 | H21A—C21—H21B | 109.5 |
| C9—C10—H10 | 119.2 | S1—C21—H21C | 109.5 |
| C12—C11—C10 | 118.28 (19) | H21A—C21—H21C | 109.5 |
| C12—C11—H11 | 120.9 | H21B—C21—H21C | 109.5 |
| C21—S1—C1—C8 | 115.0 (2) | C5—C4—C9—C14 | 152.2 (2) |
| C21—S1—C1—C2 | -67.4 (2) | C3—C4—C9—C10 | 151.49 (19) |
| C8—C1—C2—C7 | 0.0 (2) | C5—C4—C9—C10 | -28.1 (3) |
| S1—C1—C2—C7 | -178.03 (16) | C14—C9—C10—C11 | 0.9 (3) |
| C8—C1—C2—C3 | -179.1 (2) | C4—C9—C10—C11 | -178.74 (19) |
| S1—C1—C2—C3 | 2.9 (3) | C9—C10—C11—C12 | -0.2 (3) |
| C7—C2—C3—C4 | -0.8 (3) | C10—C11—C12—F1 | 179.42 (19) |
| C1—C2—C3—C4 | 178.1 (2) | C10—C11—C12—C13 | -0.2 (3) |
| C2—C3—C4—C5 | 1.7 (3) | F1—C12—C13—C14 | -179.68 (18) |
| C2—C3—C4—C9 | -177.88 (18) | C11—C12—C13—C14 | -0.1 (3) |
| C3—C4—C5—C6 | -1.4 (3) | C12—C13—C14—C9 | 0.8 (3) |
| C9—C4—C5—C6 | 178.20 (19) | C10—C9—C14—C13 | -1.2 (3) |
| C4—C5—C6—C7 | 0.1 (3) | C4—C9—C14—C13 | 178.46 (18) |
| C8—O1—C7—C6 | 179.7 (2) | C1—C8—C15—C20 | -154.5 (2) |
| C8—O1—C7—C2 | -0.3 (2) | O1—C8—C15—C20 | 24.2 (3) |
| C5—C6—C7—O1 | -179.09 (19) | C1—C8—C15—C16 | 26.1 (3) |
| C5—C6—C7—C2 | 0.9 (3) | O1—C8—C15—C16 | -155.20 (18) |
| C3—C2—C7—O1 | 179.44 (16) | C20—C15—C16—C17 | -0.1 (3) |
| C1—C2—C7—O1 | 0.2 (2) | C8—C15—C16—C17 | 179.37 (17) |
| C3—C2—C7—C6 | -0.5 (3) | C15—C16—C17—C18 | 1.1 (3) |
| C1—C2—C7—C6 | -179.78 (19) | C16—C17—C18—F2 | 179.39 (17) |
| C2—C1—C8—O1 | -0.1 (2) | C16—C17—C18—C19 | -1.3 (3) |
| S1—C1—C8—O1 | 177.79 (15) | F2—C18—C19—C20 | 179.82 (18) |
| C2—C1—C8—C15 | 178.6 (2) | C17—C18—C19—C20 | 0.6 (3) |
| S1—C1—C8—C15 | -3.5 (4) | C18—C19—C20—C15 | 0.5 (3) |
| C7—O1—C8—C1 | 0.3 (2) | C16—C15—C20—C19 | -0.8 (3) |
| C7—O1—C8—C15 | -178.75 (16) | C8—C15—C20—C19 | 179.82 (18) |
| C3—C4—C9—C14 | -28.1 (3) | | |

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

Cg is the centroid of the C15–C20 4-fluorophenyl ring.

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|------------------------------------|-------|-------------|-------------|---------------|
| C6—H6 \cdots F1 ⁱ | 0.95 | 2.45 | 3.322 (2) | 153. |
| C10—H10 \cdots Cg ⁱⁱ | 0.95 | 2.67 | 3.441 (2) | 139. |
| C17—H17 \cdots Cg ⁱⁱⁱ | 0.95 | 2.86 | 3.557 (2) | 131. |

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

Fig. 1

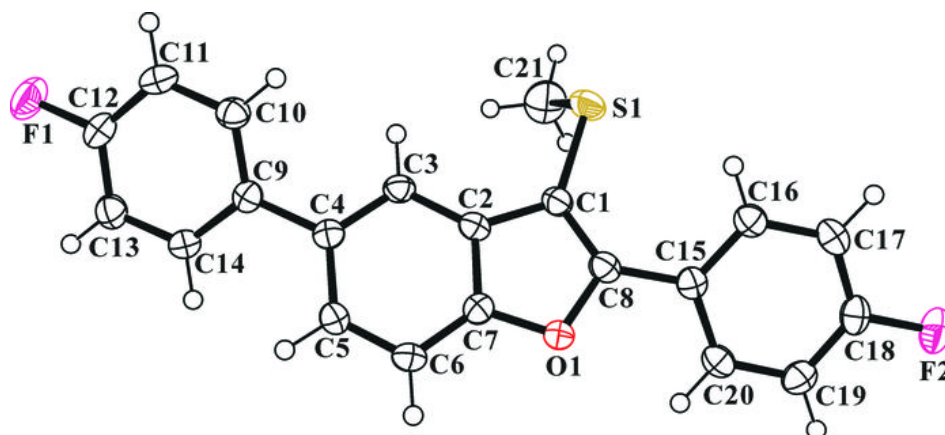


Fig. 2

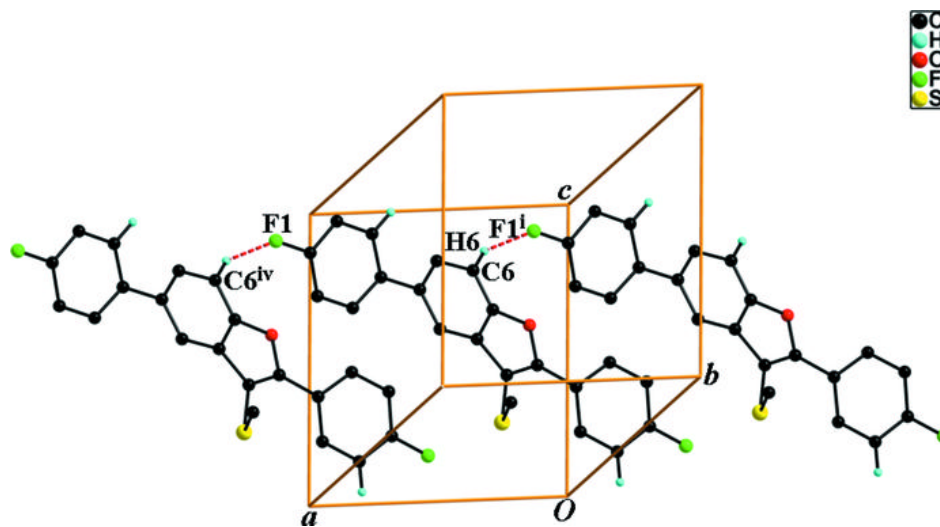


Fig. 3

