# organic compounds

# 2-(3-Fluorophenyl)-3-methylsulfanyl-5-phenyl-1-benzofuran

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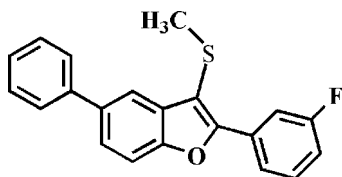Correspondence e-mail: uklee@pknu.ac.kr

In the title compound, $C_{21}H_{15}FOS$, the dihedral angles between the mean plane of the benzofuran fragment and the pendant 3-fluorophenyl and phenyl rings are 1.76 (5) and 32.29 (5)°, respectively. In the crystal, molecules are linked by a slipped $\pi$–$\pi$ interaction between the furan and benzene rings of neighbouring molecules [centroid–centroid distance = 3.665 (2) Å, interplanar distance = 3.391 (2) Å and slippage = 1.390 (2) 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 related structures, see: Choi *et al.* (2009, 2010).



## Experimental

### Crystal data

| | |
|---|---|
| $C_{21}H_{15}FOS$ | $\gamma = 80.061\ (1)°$ |
| $M_r = 334.39$ | $V = 787.82\ (3)$ Å$^3$ |
| Triclinic, $P\bar{1}$ | $Z = 2$ |
| $a = 4.7692\ (1)$ Å | Mo $K\alpha$ radiation |
| $b = 9.6442\ (2)$ Å | $\mu = 0.22$ mm$^{-1}$ |
| $c = 17.4049\ (3)$ Å | $T = 296$ K |
| $\alpha = 89.7700\ (1)°$ | $0.34 \times 0.25 \times 0.12$ mm |
| $\beta = 87.589\ (1)°$ | |

### Data collection

| | |
|---|---|
| Bruker SMART APEXII CCD diffractometer | 13895 measured reflections |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2009) | 3590 independent reflections |
| | 3234 reflections with $I > 2\sigma(I)$ |
| $T_{min} = 0.929$, $T_{max} = 0.974$ | $R_{int} = 0.023$ |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.034$ | 218 parameters |
| $wR(F^2) = 0.091$ | H-atom parameters constrained |
| $S = 1.04$ | $\Delta\rho_{max} = 0.30$ e Å$^{-3}$ |
| 3590 reflections | $\Delta\rho_{min} = -0.25$ 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: FF2033).

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**supplementary materials**

## 2-(3-Fluorophenyl)-3-methylsulfanyl-5-phenyl-1-benzofuran

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

### Comment

Recently, many compounds having a benzofuran moiety have drawn much attention due 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 benzofuranderivatives containing either 2-(4-fluorophenyl) (Choi *et al.*, 2009) or 2-(4-chlorophenyl) (Choi *et al.*, 2010) substituents, 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 (1) Å from the least-squares plane defined by the nine constituent atoms. The dihedral angles between the mean plane of the benzofuran fragment and the 4-fluorophenyl and phenyl rings are 1.76 (5)° and 32.29 (5)°, respectively. The crystal packing (Fig. 2) is stabilized by a slipped π–π interaction between the furan and benzene rings of adjacent molecules, with a Cg1···Cg2$^i$ distance of 3.665 (2) Å and an interplanar distance of 3.391 (2) Å resulting in a slippage of 1.390 (2) Å (Cg1 and Cg2 are the centroids of the C1/C2/C7/O1/C8 furan ring and the C2–C7 benzene ring, respectively).

### Experimental

Zinc chloride (273 mg, 2.0 mmol) was added to a stirred solution of 4-phenylphenol (340 mg, 2.0 mmol) and 2-chloro-2-methylsulfanyl-3'-fluoroacetophenone (437 mg, 2.0 mmol) in dichloromethane (30 mL) at room temperature, and stirring was continued at the same temperature for 1h. 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 (hexane–benzene, 5:2 v/v) to afford the title compound as a colorless solid [yield 54%, m.p. 357–358 K; $R_f$ = 0.61 (hexane–benzene, 5:2 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.

### Refinement

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. $U_{iso}$(H) =1.2$U_{eq}$(C) for aryl and 1.5$U_{eq}$(C) for methyl H atoms.
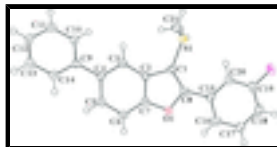
### Figures



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 small spheres of arbitrary radius.
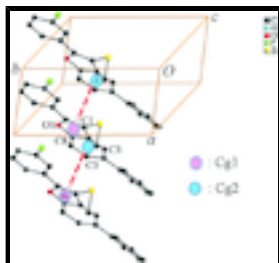
Fig. 2. A view of the π–π interactions (dotted lines) in the crystal structure of the title compound. H atoms were omitted for clarity. [Symmetry codes: (i) $x - 1, y, z$; (ii) $x + 1, y, z$.]

## 2-(3-Fluorophenyl)-3-methylsulfanyl-5-phenyl-1-benzofuran

*Crystal data*

| | |
|---|---|
| $C_{21}H_{15}FOS$ | $Z = 2$ |
| $M_r = 334.39$ | $F(000) = 348$ |
| Triclinic, $P\bar{1}$ | $D_x = 1.410$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 4.7692$ (1) Å | Cell parameters from 7407 reflections |
| $b = 9.6442$ (2) Å | $\theta = 2.3$–$27.5°$ |
| $c = 17.4049$ (3) Å | $\mu = 0.22$ mm$^{-1}$ |
| $\alpha = 89.7700$ (1)° | $T = 296$ K |
| $\beta = 87.589$ (1)° | Block, colourless |
| $\gamma = 80.061$ (1)° | $0.34 \times 0.25 \times 0.12$ mm |
| $V = 787.82$ (3) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART APEXII CCD diffractometer | 3590 independent reflections |
| Radiation source: rotating anode | 3234 reflections with $I > 2\sigma(I)$ |
| graphite multilayer | $R_{int} = 0.023$ |
| Detector resolution: 10.0 pixels mm$^{-1}$ | $\theta_{max} = 27.5°$, $\theta_{min} = 2.1°$ |
| φ and ω scans | $h = -6 \rightarrow 6$ |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2009) | $k = -12 \rightarrow 12$ |
| $T_{min} = 0.929$, $T_{max} = 0.974$ | $l = -22 \rightarrow 22$ |
| 13895 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.034$ | Hydrogen site location: difference Fourier map |
| $wR(F^2) = 0.091$ | H-atom parameters constrained |
| $S = 1.04$ | $w = 1/[\sigma^2(F_o^2) + (0.0451P)^2 + 0.3462P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 3590 reflections | $(\Delta/\sigma)_{max} < 0.001$ |

218 parameters

$\Delta\rho_{max} = 0.30$ e Å$^{-3}$

0 restraints

$\Delta\rho_{min} = -0.25$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.94952 (7) | 0.43069 (3) | 0.147672 (18) | 0.02311 (10) |
| F1 | 0.2102 (2) | 0.79398 (10) | 0.01953 (5) | 0.0391 (2) |
| O1 | 1.05781 (19) | 0.76869 (9) | 0.26561 (5) | 0.0218 (2) |
| C1 | 1.0423 (3) | 0.56199 (13) | 0.20611 (7) | 0.0196 (2) |
| C2 | 1.2552 (3) | 0.53713 (13) | 0.26345 (7) | 0.0199 (2) |
| C3 | 1.4383 (3) | 0.41893 (13) | 0.28916 (7) | 0.0198 (2) |
| H3 | 1.4391 | 0.3310 | 0.2674 | 0.024* |
| C4 | 1.6195 (3) | 0.43454 (13) | 0.34781 (7) | 0.0200 (2) |
| C5 | 1.6144 (3) | 0.56915 (14) | 0.38003 (7) | 0.0232 (3) |
| H5 | 1.7378 | 0.5787 | 0.4189 | 0.028* |
| C6 | 1.4325 (3) | 0.68749 (14) | 0.35590 (7) | 0.0238 (3) |
| H6 | 1.4295 | 0.7757 | 0.3777 | 0.029* |
| C7 | 1.2556 (3) | 0.66699 (13) | 0.29759 (7) | 0.0205 (2) |
| C8 | 0.9298 (3) | 0.70255 (13) | 0.20980 (7) | 0.0203 (2) |
| C9 | 1.8215 (3) | 0.31190 (13) | 0.37610 (7) | 0.0211 (3) |
| C10 | 1.9415 (3) | 0.20260 (14) | 0.32642 (8) | 0.0248 (3) |
| H10 | 1.8910 | 0.2055 | 0.2753 | 0.030* |
| C11 | 2.1353 (3) | 0.08960 (14) | 0.35218 (8) | 0.0308 (3) |
| H11 | 2.2143 | 0.0176 | 0.3184 | 0.037* |
| C12 | 2.2111 (4) | 0.08401 (15) | 0.42809 (9) | 0.0367 (4) |
| H12 | 2.3420 | 0.0087 | 0.4453 | 0.044* |
| C13 | 2.0914 (4) | 0.19081 (16) | 0.47824 (9) | 0.0362 (4) |
| H13 | 2.1406 | 0.1867 | 0.5294 | 0.043* |
| C14 | 1.8985 (3) | 0.30393 (15) | 0.45263 (8) | 0.0279 (3) |
| H14 | 1.8195 | 0.3753 | 0.4868 | 0.034* |
| C15 | 0.7126 (3) | 0.79758 (13) | 0.16924 (7) | 0.0212 (3) |
| C16 | 0.6597 (3) | 0.94127 (15) | 0.18697 (8) | 0.0299 (3) |
| H16 | 0.7610 | 0.9756 | 0.2250 | 0.036* |
| C17 | 0.4572 (3) | 1.03289 (16) | 0.14822 (9) | 0.0357 (3) |
| H17 | 0.4239 | 1.1281 | 0.1608 | 0.043* |

| | | | | |
|---|---|---|---|---|
| C18 | 0.3041 (3) | 0.98512 (16) | 0.09120 (8) | 0.0315 (3) |
| H18 | 0.1692 | 1.0464 | 0.0648 | 0.038* |
| C19 | 0.3592 (3) | 0.84369 (15) | 0.07508 (8) | 0.0262 (3) |
| C20 | 0.5568 (3) | 0.74876 (14) | 0.11223 (7) | 0.0237 (3) |
| H20 | 0.5859 | 0.6536 | 0.0995 | 0.028* |
| C21 | 1.2261 (3) | 0.41386 (17) | 0.07312 (9) | 0.0352 (3) |
| H21A | 1.2159 | 0.5014 | 0.0461 | 0.053* |
| H21B | 1.2017 | 0.3410 | 0.0379 | 0.053* |
| H21C | 1.4086 | 0.3902 | 0.0956 | 0.053* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.02386 (17) | 0.02130 (17) | 0.02495 (17) | −0.00512 (12) | −0.00487 (12) | −0.00323 (12) |
| F1 | 0.0392 (5) | 0.0395 (5) | 0.0387 (5) | −0.0029 (4) | −0.0205 (4) | −0.0007 (4) |
| O1 | 0.0230 (5) | 0.0190 (4) | 0.0229 (4) | −0.0008 (3) | −0.0057 (3) | −0.0021 (3) |
| C1 | 0.0188 (6) | 0.0206 (6) | 0.0196 (6) | −0.0038 (4) | −0.0018 (4) | −0.0009 (4) |
| C2 | 0.0189 (6) | 0.0217 (6) | 0.0194 (6) | −0.0048 (5) | −0.0001 (4) | −0.0014 (5) |
| C3 | 0.0204 (6) | 0.0181 (6) | 0.0212 (6) | −0.0042 (4) | −0.0001 (4) | −0.0014 (4) |
| C4 | 0.0204 (6) | 0.0192 (6) | 0.0204 (6) | −0.0033 (5) | −0.0001 (4) | 0.0004 (4) |
| C5 | 0.0248 (6) | 0.0236 (6) | 0.0214 (6) | −0.0035 (5) | −0.0054 (5) | −0.0022 (5) |
| C6 | 0.0278 (7) | 0.0193 (6) | 0.0243 (6) | −0.0029 (5) | −0.0040 (5) | −0.0048 (5) |
| C7 | 0.0204 (6) | 0.0186 (6) | 0.0217 (6) | −0.0009 (4) | −0.0021 (5) | 0.0003 (5) |
| C8 | 0.0204 (6) | 0.0222 (6) | 0.0189 (6) | −0.0051 (5) | −0.0018 (4) | −0.0016 (5) |
| C9 | 0.0208 (6) | 0.0198 (6) | 0.0235 (6) | −0.0053 (5) | −0.0033 (5) | 0.0022 (5) |
| C10 | 0.0297 (7) | 0.0203 (6) | 0.0245 (6) | −0.0038 (5) | −0.0056 (5) | 0.0008 (5) |
| C11 | 0.0365 (8) | 0.0198 (6) | 0.0342 (8) | 0.0015 (5) | −0.0069 (6) | −0.0032 (5) |
| C12 | 0.0435 (9) | 0.0221 (7) | 0.0427 (9) | 0.0034 (6) | −0.0199 (7) | 0.0010 (6) |
| C13 | 0.0486 (9) | 0.0287 (7) | 0.0307 (7) | −0.0009 (6) | −0.0183 (7) | 0.0010 (6) |
| C14 | 0.0344 (7) | 0.0241 (7) | 0.0245 (7) | −0.0015 (5) | −0.0061 (5) | −0.0022 (5) |
| C15 | 0.0189 (6) | 0.0223 (6) | 0.0219 (6) | −0.0024 (5) | 0.0002 (5) | 0.0012 (5) |
| C16 | 0.0318 (7) | 0.0243 (7) | 0.0328 (7) | −0.0010 (5) | −0.0093 (6) | −0.0027 (5) |
| C17 | 0.0408 (8) | 0.0227 (7) | 0.0413 (8) | 0.0030 (6) | −0.0113 (7) | −0.0011 (6) |
| C18 | 0.0284 (7) | 0.0310 (7) | 0.0327 (7) | 0.0030 (6) | −0.0067 (6) | 0.0060 (6) |
| C19 | 0.0229 (6) | 0.0330 (7) | 0.0233 (6) | −0.0054 (5) | −0.0049 (5) | 0.0007 (5) |
| C20 | 0.0235 (6) | 0.0235 (6) | 0.0240 (6) | −0.0031 (5) | −0.0023 (5) | 0.0000 (5) |
| C21 | 0.0333 (8) | 0.0419 (9) | 0.0319 (7) | −0.0110 (6) | 0.0015 (6) | −0.0137 (6) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| S1—C1 | 1.7537 (13) | C10—H10 | 0.9300 |
| S1—C21 | 1.7984 (15) | C11—C12 | 1.383 (2) |
| F1—C19 | 1.3597 (16) | C11—H11 | 0.9300 |
| O1—C7 | 1.3719 (14) | C12—C13 | 1.382 (2) |
| O1—C8 | 1.3830 (15) | C12—H12 | 0.9300 |
| C1—C8 | 1.3698 (17) | C13—C14 | 1.3854 (19) |
| C1—C2 | 1.4435 (17) | C13—H13 | 0.9300 |
| C2—C7 | 1.3887 (17) | C14—H14 | 0.9300 |
| C2—C3 | 1.3955 (17) | C15—C20 | 1.3946 (18) |

| | | | |
|---|---|---|---|
| C3—C4 | 1.3897 (17) | C15—C16 | 1.3984 (19) |
| C3—H3 | 0.9300 | C16—C17 | 1.387 (2) |
| C4—C5 | 1.4122 (18) | C16—H16 | 0.9300 |
| C4—C9 | 1.4873 (17) | C17—C18 | 1.383 (2) |
| C5—C6 | 1.3843 (18) | C17—H17 | 0.9300 |
| C5—H5 | 0.9300 | C18—C19 | 1.372 (2) |
| C6—C7 | 1.3829 (18) | C18—H18 | 0.9300 |
| C6—H6 | 0.9300 | C19—C20 | 1.3758 (18) |
| C8—C15 | 1.4629 (17) | C20—H20 | 0.9300 |
| C9—C10 | 1.3942 (18) | C21—H21A | 0.9600 |
| C9—C14 | 1.3948 (18) | C21—H21B | 0.9600 |
| C10—C11 | 1.3879 (18) | C21—H21C | 0.9600 |
| | | | |
| C1—S1—C21 | 101.72 (6) | C10—C11—H11 | 120.0 |
| C7—O1—C8 | 106.60 (9) | C13—C12—C11 | 119.73 (13) |
| C8—C1—C2 | 106.46 (11) | C13—C12—H12 | 120.1 |
| C8—C1—S1 | 129.09 (10) | C11—C12—H12 | 120.1 |
| C2—C1—S1 | 124.41 (9) | C12—C13—C14 | 120.36 (13) |
| C7—C2—C3 | 119.37 (11) | C12—C13—H13 | 119.8 |
| C7—C2—C1 | 105.75 (11) | C14—C13—H13 | 119.8 |
| C3—C2—C1 | 134.88 (12) | C13—C14—C9 | 120.69 (13) |
| C4—C3—C2 | 119.05 (11) | C13—C14—H14 | 119.7 |
| C4—C3—H3 | 120.5 | C9—C14—H14 | 119.7 |
| C2—C3—H3 | 120.5 | C20—C15—C16 | 118.60 (12) |
| C3—C4—C5 | 119.45 (12) | C20—C15—C8 | 121.58 (12) |
| C3—C4—C9 | 120.87 (11) | C16—C15—C8 | 119.82 (12) |
| C5—C4—C9 | 119.67 (11) | C17—C16—C15 | 120.44 (13) |
| C6—C5—C4 | 122.43 (12) | C17—C16—H16 | 119.8 |
| C6—C5—H5 | 118.8 | C15—C16—H16 | 119.8 |
| C4—C5—H5 | 118.8 | C18—C17—C16 | 121.14 (14) |
| C7—C6—C5 | 116.14 (12) | C18—C17—H17 | 119.4 |
| C7—C6—H6 | 121.9 | C16—C17—H17 | 119.4 |
| C5—C6—H6 | 121.9 | C19—C18—C17 | 117.29 (13) |
| O1—C7—C6 | 125.91 (11) | C19—C18—H18 | 121.4 |
| O1—C7—C2 | 110.53 (11) | C17—C18—H18 | 121.4 |
| C6—C7—C2 | 123.56 (12) | F1—C19—C18 | 118.41 (12) |
| C1—C8—O1 | 110.66 (11) | F1—C19—C20 | 117.96 (13) |
| C1—C8—C15 | 135.74 (12) | C18—C19—C20 | 123.63 (13) |
| O1—C8—C15 | 113.59 (11) | C19—C20—C15 | 118.90 (12) |
| C10—C9—C14 | 118.30 (12) | C19—C20—H20 | 120.6 |
| C10—C9—C4 | 120.71 (11) | C15—C20—H20 | 120.6 |
| C14—C9—C4 | 120.98 (12) | S1—C21—H21A | 109.5 |
| C11—C10—C9 | 120.88 (12) | S1—C21—H21B | 109.5 |
| C11—C10—H10 | 119.6 | H21A—C21—H21B | 109.5 |
| C9—C10—H10 | 119.6 | S1—C21—H21C | 109.5 |
| C12—C11—C10 | 120.04 (13) | H21A—C21—H21C | 109.5 |
| C12—C11—H11 | 120.0 | H21B—C21—H21C | 109.5 |
| | | | |
| C21—S1—C1—C8 | 100.68 (13) | C3—C4—C9—C10 | 32.27 (18) |
| C21—S1—C1—C2 | −81.81 (12) | C5—C4—C9—C10 | −146.70 (13) |

| | | | |
|---|---|---|---|
| C8—C1—C2—C7 | −0.32 (13) | C3—C4—C9—C14 | −148.48 (13) |
| S1—C1—C2—C7 | −178.30 (9) | C5—C4—C9—C14 | 32.55 (18) |
| C8—C1—C2—C3 | 178.54 (13) | C14—C9—C10—C11 | −0.8 (2) |
| S1—C1—C2—C3 | 0.6 (2) | C4—C9—C10—C11 | 178.47 (13) |
| C7—C2—C3—C4 | −0.78 (18) | C9—C10—C11—C12 | 0.3 (2) |
| C1—C2—C3—C4 | −179.52 (13) | C10—C11—C12—C13 | 0.5 (2) |
| C2—C3—C4—C5 | 0.00 (18) | C11—C12—C13—C14 | −0.7 (3) |
| C2—C3—C4—C9 | −178.97 (11) | C12—C13—C14—C9 | 0.1 (2) |
| C3—C4—C5—C6 | 0.65 (19) | C10—C9—C14—C13 | 0.6 (2) |
| C9—C4—C5—C6 | 179.63 (12) | C4—C9—C14—C13 | −178.66 (14) |
| C4—C5—C6—C7 | −0.48 (19) | C1—C8—C15—C20 | 2.0 (2) |
| C8—O1—C7—C6 | −179.95 (12) | O1—C8—C15—C20 | −178.56 (11) |
| C8—O1—C7—C2 | −0.27 (13) | C1—C8—C15—C16 | −177.34 (14) |
| C5—C6—C7—O1 | 179.30 (12) | O1—C8—C15—C16 | 2.05 (17) |
| C5—C6—C7—C2 | −0.4 (2) | C20—C15—C16—C17 | −0.3 (2) |
| C3—C2—C7—O1 | −178.71 (10) | C8—C15—C16—C17 | 179.10 (13) |
| C1—C2—C7—O1 | 0.36 (14) | C15—C16—C17—C18 | −0.3 (2) |
| C3—C2—C7—C6 | 0.99 (19) | C16—C17—C18—C19 | 0.5 (2) |
| C1—C2—C7—C6 | −179.94 (12) | C17—C18—C19—F1 | 179.64 (13) |
| C2—C1—C8—O1 | 0.17 (14) | C17—C18—C19—C20 | −0.1 (2) |
| S1—C1—C8—O1 | 178.03 (9) | F1—C19—C20—C15 | 179.80 (11) |
| C2—C1—C8—C15 | 179.58 (14) | C18—C19—C20—C15 | −0.4 (2) |
| S1—C1—C8—C15 | −2.6 (2) | C16—C15—C20—C19 | 0.63 (19) |
| C7—O1—C8—C1 | 0.05 (13) | C8—C15—C20—C19 | −178.76 (12) |
| C7—O1—C8—C15 | −179.50 (10) | | |

**Fig. 1**

**Fig. 2**