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2-(3-Fluorophenyl)-3-methylsulfanyl-5-phenyl-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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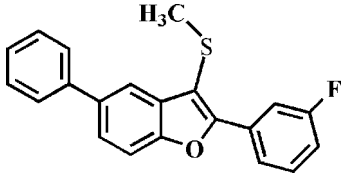
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.034; wR factor = 0.091; data-to-parameter ratio = 16.5.

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 π–π 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

$C_{21}H_{15}FOS$
M_r = 334.39
Triclinic, $P\overline{1}$
a = 4.7692 (1) Å
b = 9.6442 (2) Å
c = 17.4049 (3) Å
α = 89.7700 (1)°
β = 87.589 (1)°
γ = 80.061 (1)°
V = 787.82 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 296 K
0.34 × 0.25 × 0.12 mm

Data collection

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

Refinement

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

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

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S1. 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).

S2. 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.

S3. 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) =1.2U_{eq}(C) for aryl and 1.5U_{eq}(C) for methyl H atoms.

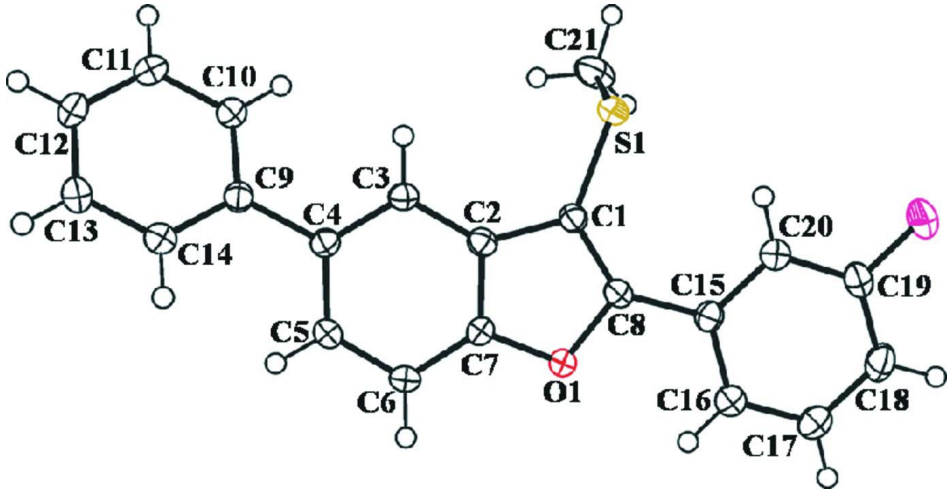

Figure 1

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 small spheres of arbitrary radius.

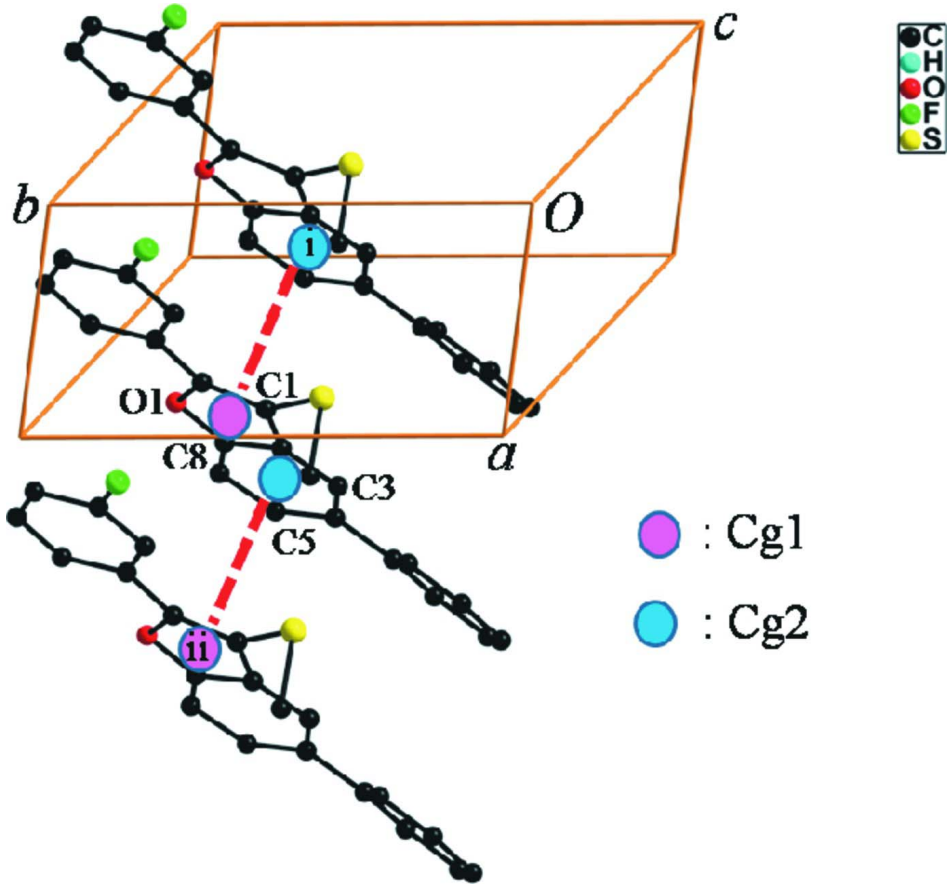

Figure 2

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.]

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$C_{21}H_{15}FOS$
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Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 4.7692$ (1) Å
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$\alpha = 89.7700$ (1)°
$\beta = 87.589$ (1)°
$\gamma = 80.061$ (1)°
$V = 787.82$ (3) Å^3
$Z = 2$
$F(000) = 348$
$D_x = 1.410$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7407 reflections
$\theta = 2.3$–$27.5°$
$\mu = 0.22$ mm^{-1}
$T = 296$ K
Block, colourless
0.34 × 0.25 × 0.12 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)
$T_{min} = 0.929$, $T_{max} = 0.974$
13895 measured reflections
3590 independent reflections
3234 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.1°$
$h = -6 \rightarrow 6$
$k = -12 \rightarrow 12$
$l = -22 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.091$
$S = 1.04$
3590 reflections
218 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
$w = 1/[\sigma^2(F_o^2) + (0.0451P)^2 + 0.3462P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ 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 $F^2 > 2$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 (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 (Å²)

	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, º)

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)		