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1,2-Bis[5-(4-cyanophenyl)-2-methyl-3-thienyl]-3,3,4,4,5,5-hexafluorocyclopent-1-ene: a photochromic diarylethene compound

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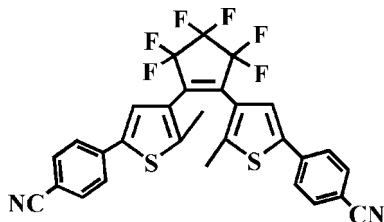
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Key indicators: single-crystal X-ray study; $T = 113$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.058; wR factor = 0.146; data-to-parameter ratio = 13.5.

The molecules of the title compound, $\text{C}_{29}\text{H}_{16}\text{F}_6\text{N}_2\text{S}_2$, a photochromic dithienylethene with 4-cyanophenyl substituents, adopt an antiparallel arrangement that is responsible for photoactivity. The molecule lies on a twofold rotation axis. The dihedral angle between the nearly planar cyclopentenyl and heteroaryl rings is $142.5(3)^\circ$, and that between the heteroaryl and benzene rings is $22.4(3)^\circ$. The distance between the heteroaryl rings of adjacent molecules is $3.601(2)$ Å, indicating a π - π interaction.

Related literature

For a review of dithienylethylenes as photochromic compounds, see: Irie (2000). For phenyl-substituted derivatives, see: Pu, Liu *et al.* (2005); Pu, Yang *et al.* (2005). For another similar structure, see: Kobatake *et al.* (2004). For the manifestation of possible photochromic activity in relation to the conformation, see: Woodward & Hoffmann (1970).



Experimental

Crystal data

$\text{C}_{29}\text{H}_{16}\text{F}_6\text{N}_2\text{S}_2$
 $M_r = 570.56$
Monoclinic, $C2/c$
 $a = 24.987(10)$ Å
 $b = 9.276(4)$ Å
 $c = 10.774(4)$ Å
 $\beta = 95.911(7)^\circ$
 $V = 2483.8(17)$ Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.28$ mm⁻¹
 $T = 113(2)$ K
 $0.36 \times 0.20 \times 0.10$ mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan (Jacobson, 1998)
 $T_{\min} = 0.905$, $T_{\max} = 0.972$
9917 measured reflections
2437 independent reflections
2130 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.032$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.057$
 $wR(F^2) = 0.145$
 $S = 1.06$
2437 reflections
180 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.90$ e Å⁻³
 $\Delta\rho_{\min} = -0.65$ e Å⁻³

Data collection: *CrystalClear* (Rigaku/MSC, 2001); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *CrystalStructure*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2448).

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1,2-Bis[5-(4-cyanophenyl)-2-methyl-3-thienyl]-3,3,4,4,5,5-hexafluorocyclopent-1-ene: a photochromic diarylethene compound

Gang Liu, Qidong Tu, Qing Zhang, Congbin Fan and Tianshe Yang

S1. Comment

Dithienylethenes are the most promising organic photochromic compounds for photoelectronic devices (Irie, 2000). Dithienylethenes bearing terminal phenyl groups are of special interest, because phenyl group can be substituted by many electron-donating or electron-withdrawing groups that influence the properties (Pu, Yang, Xu *et al.*, 2005). In order to investigate the substituent effect at the *para*-position on the photochemical properties, we have now synthesized the title compound, (Ia), and its structure is presented in this paper.

To the best of our knowledge, this is the first symmetrical dithienylethene compound with phenyl groups bearing *para* substituent. The molecular structure of (Ia) is shown in Fig. 1 and selected geometric parameters are given in Table 1.

The molecule contains two thiophene rings substituted by two *para*-cyanophenyl rings in a photoactive antiparallel conformation. In the cyclopent-1-ene ring, the C12=C12A bond is clearly a double bond, and the other bonds in the ring are clearly single bonds (see Table 1). The two thiophene rings are linked by the C12=C12A double bond. The two methyl groups are located on different sides of the double bond and are thus *trans* with respect to the double bond. Such a configuration is crucial for the compound to exhibit photochromic and photoinduced properties (Woodward & Hoffmann, 1970). The dihedral angles between the least-squares plane of the atoms of the central cyclopent-1-ene ring and the adjacent thiophene rings are 142.5 (3)°, and those between thiophene rings and the adjacent benzene rings are both 22.4 (3)°. The distance between the two reactive C atoms (C4_C4A) is 3.601 (2) Å. This distance indicates that the crystal can undergo photochromism in the crystalline phase because the photochromic reactivity of crystals depends on the distance between the reactive C atoms being less than 4.2 Å (Kobatake *et al.*, 2004).

Upon irradiation with 313 nm light, colorless single crystals of (Ia) turned to blue rapidly, and the blue color remained stable in the dark. When the blue crystals were dissolved in hexane, the solution also remained blue. The absorption maximum of this solution is observed at a wavelength of 596 nm, consistent with the presence of the closed-ring isomer, (Ib). This result suggests that the title compound undergoes a photochromic reaction to produce the closed-ring molecule of (Ib) in the single-crystal phase. We have not, so far, been able to determine the crystal structure of (Ib). Furthermore, upon irradiation with wavelengths longer than 450 nm, the blue crystal changes back to colorless, and the absorption spectrum of a hexane solution of the colorless crystals is the same as that of a solution of the open-ring form, (Ia), with the absorption maximum at 314 nm.

S2. Experimental

The title compound was originally derived from 2-methylthiophene(1). 3-Bromo-2-methyl-5-(4-cyanophenyl)thiophene, (4) (4.60 g, 16.5 mmol), in 78.8% yield was synthesized by reacting (3) (4.62 g, 20.9 mmol) (Pu, Liu *et al.*, 2005) with 4-cyano-brombenzene (3.82 g, 21.0 mmol) in the presence of Pd(PPh₃)₄ (0.5 g) and Na₂CO₃ (2 mol/L, 30 ml) in tetrahydrofuran (THF, 80 ml) for 16 h at 343 K. To a stirred THF solution (60 ml) of (4) (2.21 g, 7.96 mmol) 3.3 ml of n-

BuLi/hexane solution (2.5 M, 8.2 mmol) was slowly added at 195 K under a nitrogen atmosphere. 30 min later, octafluorocyclopentene (0.54 ml, 4.0 mmol) was added and the mixture was stirred for 2 h. The reaction mixture was extracted with diethyl ether and evaporated *in vacuo*, then purified by column chromatography (petroleum ether) to give the title compound (1.21 g, 2.12 mmol) in 53.3% yield. The compound crystallized from hexane at room temperature and produced single crystals suitable for X-ray analysis. The structure of (Ia) was confirmed by melting point, IR and NMR. Analysis calculated for $C_{29}H_{16}F_6N_2S_2$, m.p.: 485.7 K 1H NMR (400 MHz, $CDCl_3$) δ 2.03 (s, 6H), δ 7.41 (s, 2H), δ 7.64, 7.70 (d, 8H, $J = 8.0$ Hz); ^{13}C NMR (400 MHz, $CDCl_3$) δ 14.67, 111.33, 118.47, 124.41, 125.87, 126.28, 132.86, 137.34, 140.20, 143.42; IR (n, KBr, cm^{-1}): 743, 831, 846, 887, 987, 1054, 1108, 1184, 1267, 1309, 1338, 1385, 1413, 1438, 1438, 1508, 1551, 1603, 1633, 2223.

S3. Refinement

H atoms were positioned theoretically and allowed to ride on their parent atoms in the final refinement [$C-H = 0.93-0.96 \text{ \AA}$ and $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(\text{methyl } C)$]. The methyl groups were treated as rigid groups and allowed to rotate about the $C-C$ bond.

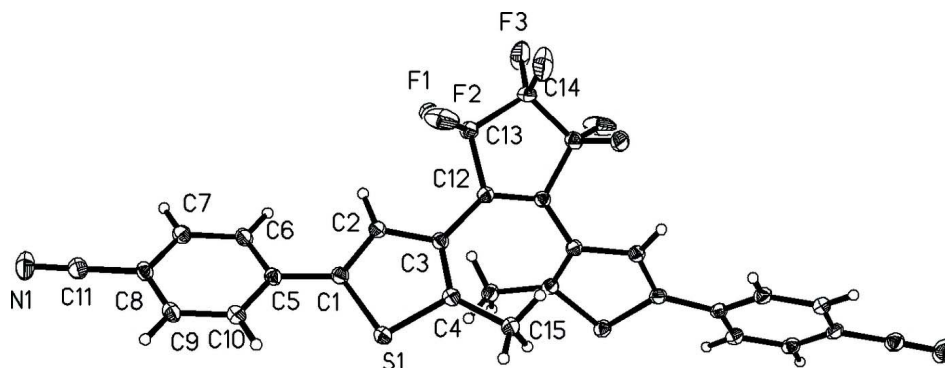


Figure 1

The molecular structure of (Ia) with 35% probability ellipsoids, showing the atomic numbering scheme.

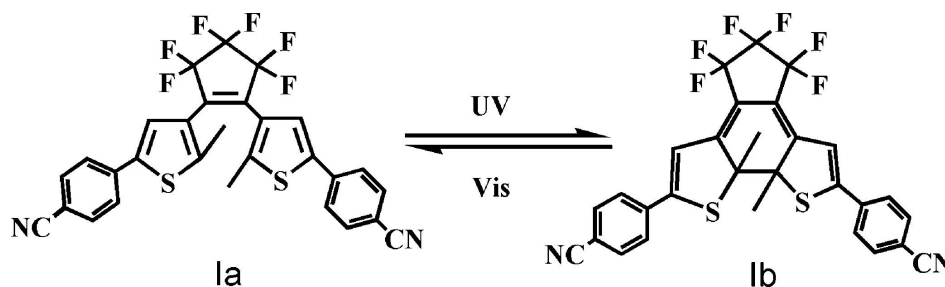
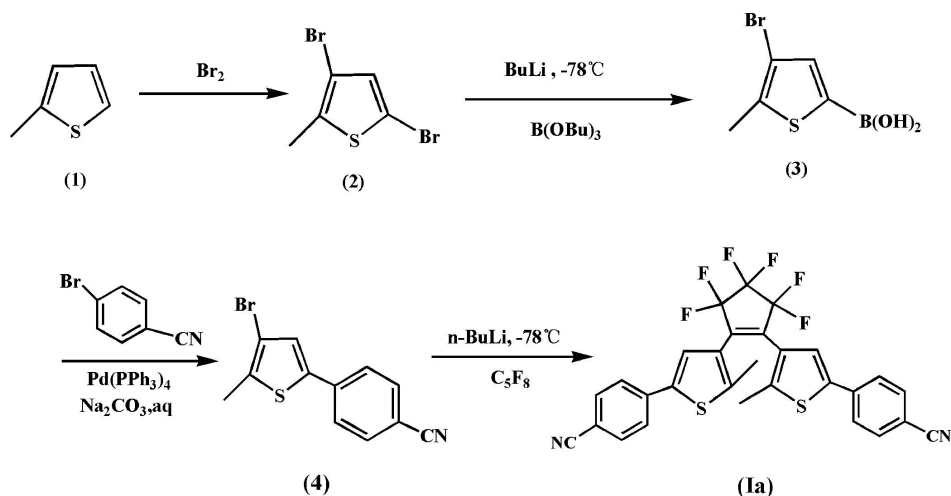


Figure 2

Interconversion of compound (Ia) and compound (Ib).


Figure 3

Synthetical method of compound (1a).

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Crystal data
 $\text{C}_{29}\text{H}_{16}\text{F}_6\text{N}_2\text{S}_2$
 $M_r = 570.56$

 Monoclinic, $C2/c$

 Hall symbol: $-C2yc$
 $a = 24.987(10) \text{ \AA}$
 $b = 9.276(4) \text{ \AA}$
 $c = 10.774(4) \text{ \AA}$
 $\beta = 95.911(7)^\circ$
 $V = 2483.8(17) \text{ \AA}^3$
 $Z = 4$
 $F(000) = 1160$
 $D_x = 1.526 \text{ Mg m}^{-3}$

 Mo $K\alpha$ radiation, $\lambda = 0.71070 \text{ \AA}$

Cell parameters from 3563 reflections

 $\theta = 1.6\text{--}27.9^\circ$
 $\mu = 0.28 \text{ mm}^{-1}$
 $T = 113 \text{ K}$

Block, colorless

 $0.36 \times 0.20 \times 0.10 \text{ mm}$
Data collection

 Rigaku Saturn
diffractometer

Radiation source: rotating anode

Confocal monochromator

 Detector resolution: $7.31 \text{ pixels mm}^{-1}$
 ω scans

Absorption correction: multi-scan

(Jacobson, 1998)

 $T_{\min} = 0.905$, $T_{\max} = 0.972$

9917 measured reflections

2437 independent reflections

 2130 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.032$
 $\theta_{\max} = 26.0^\circ$, $\theta_{\min} = 1.6^\circ$
 $h = -30 \rightarrow 30$
 $k = -11 \rightarrow 11$
 $l = -12 \rightarrow 13$
Refinement

 Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.057$
 $wR(F^2) = 0.145$
 $S = 1.07$

2437 reflections

180 parameters

0 restraints

 Primary atom site location: structure-invariant
direct methods

 Secondary atom site location: difference Fourier
map

 Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0692P)^2 + 6.3864P]$

 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.90 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.65 \text{ e \AA}^{-3}$

Extinction correction: *SHELXL97* (Sheldrick, 2008), $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0031 (9)

Special details

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 $F^2 > \sigma(F^2)$ 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	0.12440 (3)	0.06080 (7)	0.81522 (6)	0.0293 (2)
F1	0.04313 (8)	0.57014 (18)	0.94258 (16)	0.0469 (5)
F2	0.09200 (7)	0.57943 (19)	0.7907 (2)	0.0607 (7)
F3	-0.02249 (10)	0.7331 (3)	0.8302 (2)	0.0846 (10)
N1	0.34207 (11)	0.1164 (3)	1.4057 (3)	0.0492 (7)
C1	0.13504 (10)	0.1761 (3)	0.9418 (2)	0.0252 (6)
C2	0.09893 (10)	0.2871 (3)	0.9294 (2)	0.0248 (6)
H2	0.0981	0.3621	0.9893	0.030*
C3	0.06264 (10)	0.2802 (3)	0.8183 (2)	0.0244 (6)
C4	0.07183 (10)	0.1622 (3)	0.7454 (2)	0.0270 (6)
C5	0.17915 (10)	0.1560 (3)	1.0408 (2)	0.0248 (6)
C6	0.17718 (11)	0.2247 (3)	1.1548 (2)	0.0281 (6)
H6	0.1462	0.2791	1.1693	0.034*
C7	0.21958 (11)	0.2150 (3)	1.2473 (3)	0.0308 (6)
H7	0.2177	0.2624	1.3248	0.037*
C8	0.26506 (10)	0.1355 (3)	1.2265 (3)	0.0287 (6)
C9	0.26789 (11)	0.0656 (3)	1.1132 (3)	0.0292 (6)
H9	0.2990	0.0118	1.0988	0.035*
C10	0.22495 (11)	0.0750 (3)	1.0215 (3)	0.0286 (6)
H10	0.2265	0.0260	0.9445	0.034*
C11	0.30895 (11)	0.1252 (3)	1.3245 (3)	0.0350 (7)
C12	0.02472 (10)	0.3973 (3)	0.7823 (2)	0.0228 (5)
C13	0.04203 (10)	0.5483 (3)	0.8172 (3)	0.0274 (6)
C14	0.0000	0.6490 (4)	0.7500	0.0306 (8)
C15	0.04599 (12)	0.1178 (3)	0.6201 (3)	0.0331 (6)
H15A	0.0714	0.0602	0.5775	0.040*
H15B	0.0358	0.2039	0.5704	0.040*
H15C	0.0138	0.0603	0.6302	0.040*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0312 (4)	0.0264 (4)	0.0297 (4)	0.0058 (3)	-0.0006 (3)	-0.0016 (3)
F1	0.0697 (13)	0.0316 (9)	0.0346 (10)	0.0099 (8)	-0.0174 (9)	-0.0094 (7)
F2	0.0327 (10)	0.0317 (10)	0.122 (2)	-0.0050 (8)	0.0302 (11)	0.0038 (11)
F3	0.0843 (17)	0.0847 (17)	0.0741 (15)	0.0586 (14)	-0.0430 (13)	-0.0557 (13)
N1	0.0378 (15)	0.0602 (18)	0.0466 (16)	-0.0076 (13)	-0.0110 (12)	0.0141 (14)

C1	0.0246 (12)	0.0227 (12)	0.0283 (13)	0.0003 (10)	0.0023 (10)	0.0013 (10)
C2	0.0240 (12)	0.0234 (12)	0.0269 (13)	0.0005 (10)	0.0017 (10)	0.0004 (10)
C3	0.0232 (12)	0.0235 (13)	0.0263 (13)	-0.0004 (10)	0.0012 (10)	0.0023 (10)
C4	0.0277 (13)	0.0263 (13)	0.0268 (13)	0.0018 (10)	0.0012 (10)	0.0016 (11)
C5	0.0233 (12)	0.0221 (12)	0.0289 (13)	-0.0006 (10)	0.0016 (10)	0.0044 (10)
C6	0.0272 (13)	0.0262 (13)	0.0306 (14)	0.0038 (10)	0.0011 (10)	0.0026 (11)
C7	0.0357 (15)	0.0266 (14)	0.0292 (14)	-0.0003 (11)	-0.0012 (11)	0.0032 (11)
C8	0.0260 (13)	0.0267 (13)	0.0324 (14)	-0.0014 (10)	-0.0023 (11)	0.0096 (11)
C9	0.0229 (13)	0.0280 (14)	0.0366 (15)	0.0022 (10)	0.0022 (11)	0.0064 (11)
C10	0.0282 (13)	0.0275 (13)	0.0301 (14)	0.0022 (10)	0.0033 (11)	0.0025 (11)
C11	0.0304 (14)	0.0348 (15)	0.0393 (16)	-0.0022 (12)	0.0007 (13)	0.0072 (13)
C12	0.0249 (12)	0.0219 (12)	0.0216 (12)	-0.0018 (10)	0.0032 (10)	0.0007 (10)
C13	0.0218 (13)	0.0261 (13)	0.0342 (14)	-0.0021 (10)	0.0027 (11)	-0.0006 (11)
C14	0.038 (2)	0.0211 (18)	0.032 (2)	0.000	-0.0003 (16)	0.000
C15	0.0375 (15)	0.0310 (15)	0.0292 (14)	0.0076 (12)	-0.0038 (12)	-0.0051 (12)

Geometric parameters (Å, °)

S1—C4	1.724 (3)	C6—H6	0.9500
S1—C1	1.732 (3)	C7—C8	1.392 (4)
F1—C13	1.363 (3)	C7—H7	0.9500
F2—C13	1.341 (3)	C8—C9	1.390 (4)
F3—C14	1.331 (3)	C8—C11	1.446 (4)
N1—C11	1.144 (4)	C9—C10	1.384 (4)
C1—C2	1.367 (4)	C9—H9	0.9500
C1—C5	1.465 (3)	C10—H10	0.9500
C2—C3	1.427 (4)	C12—C12 ⁱ	1.354 (5)
C2—H2	0.9500	C12—C13	1.502 (3)
C3—C4	1.380 (4)	C13—C14	1.531 (3)
C3—C12	1.467 (3)	C14—F3 ⁱ	1.331 (3)
C4—C15	1.493 (4)	C14—C13 ⁱ	1.531 (3)
C5—C6	1.389 (4)	C15—H15A	0.9800
C5—C10	1.402 (4)	C15—H15B	0.9800
C6—C7	1.380 (4)	C15—H15C	0.9800
C4—S1—C1	93.15 (13)	C8—C9—H9	120.3
C2—C1—C5	127.3 (2)	C9—C10—C5	120.8 (3)
C2—C1—S1	110.0 (2)	C9—C10—H10	119.6
C5—C1—S1	122.54 (19)	C5—C10—H10	119.6
C1—C2—C3	113.8 (2)	N1—C11—C8	177.0 (3)
C1—C2—H2	123.1	C12 ⁱ —C12—C3	131.76 (14)
C3—C2—H2	123.1	C12 ⁱ —C12—C13	110.66 (14)
C4—C3—C2	112.6 (2)	C3—C12—C13	117.6 (2)
C4—C3—C12	125.3 (2)	F2—C13—F1	104.8 (2)
C2—C3—C12	121.7 (2)	F2—C13—C12	113.5 (2)
C3—C4—C15	130.6 (2)	F1—C13—C12	111.3 (2)
C3—C4—S1	110.39 (19)	F2—C13—C14	112.1 (2)
C15—C4—S1	118.9 (2)	F1—C13—C14	108.70 (19)

C6—C5—C10	118.7 (2)	C12—C13—C14	106.5 (2)
C6—C5—C1	119.6 (2)	F3 ⁱ —C14—F3	108.2 (4)
C10—C5—C1	121.6 (2)	F3 ⁱ —C14—C13 ⁱ	111.45 (14)
C7—C6—C5	120.9 (2)	F3—C14—C13 ⁱ	110.49 (15)
C7—C6—H6	119.5	F3 ⁱ —C14—C13	110.49 (15)
C5—C6—H6	119.5	F3—C14—C13	111.45 (14)
C6—C7—C8	119.8 (3)	C13 ⁱ —C14—C13	104.8 (3)
C6—C7—H7	120.1	C4—C15—H15A	109.5
C8—C7—H7	120.1	C4—C15—H15B	109.5
C9—C8—C7	120.3 (2)	H15A—C15—H15B	109.5
C9—C8—C11	120.5 (2)	C4—C15—H15C	109.5
C7—C8—C11	119.2 (3)	H15A—C15—H15C	109.5
C10—C9—C8	119.4 (2)	H15B—C15—H15C	109.5
C10—C9—H9	120.3		
C4—S1—C1—C2	0.4 (2)	C8—C9—C10—C5	1.1 (4)
C4—S1—C1—C5	-176.3 (2)	C6—C5—C10—C9	-1.2 (4)
C5—C1—C2—C3	176.4 (2)	C1—C5—C10—C9	175.4 (2)
S1—C1—C2—C3	-0.1 (3)	C4—C3—C12—C12 ⁱ	37.9 (5)
C1—C2—C3—C4	-0.3 (3)	C2—C3—C12—C12 ⁱ	-149.8 (3)
C1—C2—C3—C12	-173.6 (2)	C4—C3—C12—C13	-140.0 (3)
C2—C3—C4—C15	-176.1 (3)	C2—C3—C12—C13	32.3 (3)
C12—C3—C4—C15	-3.2 (5)	C12 ⁱ —C12—C13—F2	-131.7 (3)
C2—C3—C4—S1	0.6 (3)	C3—C12—C13—F2	46.7 (3)
C12—C3—C4—S1	173.5 (2)	C12 ⁱ —C12—C13—F1	110.5 (3)
C1—S1—C4—C3	-0.6 (2)	C3—C12—C13—F1	-71.2 (3)
C1—S1—C4—C15	176.6 (2)	C12 ⁱ —C12—C13—C14	-7.9 (3)
C2—C1—C5—C6	21.9 (4)	C3—C12—C13—C14	170.46 (19)
S1—C1—C5—C6	-162.0 (2)	F2—C13—C14—F3 ⁱ	7.2 (3)
C2—C1—C5—C10	-154.7 (3)	F1—C13—C14—F3 ⁱ	122.5 (2)
S1—C1—C5—C10	21.4 (3)	C12—C13—C14—F3 ⁱ	-117.5 (3)
C10—C5—C6—C7	0.6 (4)	F2—C13—C14—F3	-113.2 (3)
C1—C5—C6—C7	-176.0 (2)	F1—C13—C14—F3	2.2 (3)
C5—C6—C7—C8	0.0 (4)	C12—C13—C14—F3	122.2 (3)
C6—C7—C8—C9	-0.1 (4)	F2—C13—C14—C13 ⁱ	127.3 (3)
C6—C7—C8—C11	-179.4 (3)	F1—C13—C14—C13 ⁱ	-117.3 (2)
C7—C8—C9—C10	-0.4 (4)	C12—C13—C14—C13 ⁱ	2.69 (11)
C11—C8—C9—C10	178.9 (2)		

Symmetry code: (i) $-x, y, -z+3/2$.