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3,3,4,4,5,5-Hexafluoro-1,2-bis(5-formyl-2-methylsulfanyl-3-thienyl)cyclopent-1-ene

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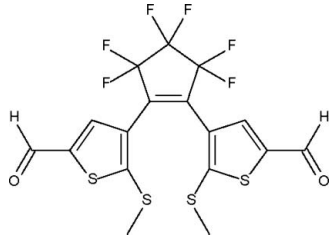
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.049; wR factor = 0.141; data-to-parameter ratio = 15.4.

In the crystal structure of the title diarylethylene compound, $C_{17}H_{10}F_6O_2S_4$, the two 3-thienyl substituents are aligned at 44.9 (1) and 40.2 (1)° with respect to the –C—C═C—C– fragment of the central cyclopentenyl ring. The five-membered cyclopentenyl ring adopts an envelope conformation. The flap atom of this ring and the two F atoms bonded to it are disordered over two positions with occupancies 0.810 (5)/0.190 (5).

Related literature

See Liu *et al.* (2008) for background literature on this class of photochromic diarylethene compounds.



Experimental

Crystal data

$C_{17}H_{10}F_6O_2S_4$
M_r = 488.49
Monoclinic, $P2_1/c$
a = 10.7640 (8) Å
b = 11.8807 (9) Å
c = 15.486 (1) Å
β = 93.407 (1)°
V = 1976.9 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.55 mm^{-1}
T = 291 (2) K
0.38 × 0.29 × 0.28 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.830, T_{max} = 0.858
12872 measured reflections
4488 independent reflections
3623 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.140
S = 1.03
4488 reflections
292 parameters
32 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.70 e Å^{-3}

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2419).

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supplementary materials

Acta Cryst. (2008). E**64**, o1007 [**doi:10.1107/S1600536808012695**]

3,3,4,4,5,5-Hexafluoro-1,2-bis(5-formyl-2-methylsulfanyl-3-thienyl)cyclopent-1-ene

Q. Tu, C. Fan, G. Liu, M. Li and S. W. Ng

Comment

A previous study describes the structure of a photochromic compound, 1,2-bis[5-(4-cyanophenyl)-2-methyl-3-thienyl]-3,3,4,4,5,5-\ hexafluorocyclopent-1-ene (Liu *et al.*, 2008). The study is extended to the title compound (Scheme I, Fig. 1). The diarylethylene compound, $C_{17}H_{10}F_6O_2S_4$, has its 3-thienyl substituents aligned at 41.4 (1) and 43.5 (1)° with respect to the central cyclopentenyl ring, which is almost flat.

Experimental

5-(Methylthio)thiophene-2-carbaldehyde was brominated to 4-bromo-5-(methylthio)thiophene-2-carbaldehyde at 273 K. The carbonyl group was converted to an acetal group by the treatment of the aldehyde (3.2 g, 13.6 mmol) with glycol (4.2 g, 70 mmol) catalyzed by *p*-toluenesulfonic acid (0.07 g, 0.41 mmol) in benzene (150 ml). The resulting compound (3.82 g, 13.4 mmol) in THF (50 ml) was reacted with 2.5 *M* butyllithium (5.34 ml) at 195 K under a nitrogen atmosphere. Octafluorocyclopentene (0.91 ml, 6.68 mmol) was added, and the reaction was quenched by water. Column chromatography on silica gave 3,3,4,4,5,5-hexafluoro- 1,2-bis[5-(1,3-dioxolan-2-yl)-2-methylthio-3-thienyl]cyclopent-1-ene (1.2 g, 2.00 mmol). The compound was hydrolyzed to give the title compound in 90% yield. Yellow crystals were obtained by the vapor diffusion of chloroform and hexane (1:1). C and H elemental analysis, Calc. for $C_{17}H_{10}F_6O_2S_4$ (%): C 41.80, H 2.06; found: C 41.73, H 2.07%.

Refinement

The cyclopentenyl ring has a flat –C–C=C–C– fragment; the fifth member comprises the flap of the envelop, and is disordered. Restraints were imposed so that the ring adopts such a conformation; the 1,2-related atoms, C6/C7 and C7/C8 were restrained to 1.54±0.01 Å, and the 1,3-related C6/C8 atoms to 2.51±0.01 Å. The four C–F distances were restrained to within 0.01 Å of each other; the anisotropic temperature factors of the minor component atoms were restrained to be nearly isotropic. The disorder refined to a 81 (1):19 ratio. The final difference Fourier map had a large peak in the vicinity of the ordered fluorine atoms.

Hydrogen atoms were positioned geometrically (C–H 0.93 to 0.96 Å)] and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2 to 1.5 times the U_{eq} of the parent atom.

Figures

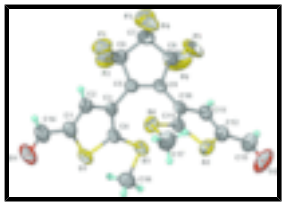

Fig. 1. Thermal ellipsoid plot (Barbour) at the 50% probability level. Hydrogen atoms are shown as spheres of arbitrary radii; the minor disorder component is not shown.

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Crystal data

$C_{17}H_{10}F_6O_2S_4$	F_{000} = 984
M_r = 488.49	D_x = 1.641 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 5293 reflections
a = 10.7640 (8) Å	θ = 2.6–28.2º
b = 11.8807 (9) Å	μ = 0.55 mm^{-1}
c = 15.486 (1) Å	T = 291 (2) K
β = 93.407 (1)º	Block, yellow
V = 1976.9 (2) Å^3	0.38 × 0.29 × 0.28 mm
Z = 4	

Data collection

Bruker APEXII diffractometer	4488 independent reflections
Radiation source: fine-focus sealed tube	3623 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.017
T = 291(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 2.6º
Absorption correction: Multi-scan (SADABS; Sheldrick, 1996)	h = −13→13
T_{min} = 0.830, T_{max} = 0.858	k = −15→15
12872 measured reflections	l = −20→19

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.048	H-atom parameters constrained
$wR(F^2)$ = 0.140	$w = 1/[\sigma^2(F_o^2) + (0.0719P)^2 + 1.6843P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max}$ = 0.001

4488 reflections	$\Delta\rho_{max}$ = 1.28 e Å^{-3}
292 parameters	$\Delta\rho_{min}$ = −0.70 e Å^{-3}
32 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.85945 (7)	0.33347 (7)	0.64145 (5)	0.0517 (2)	
S2	0.88965 (7)	−0.05788 (6)	0.39840 (5)	0.0492 (2)	
S3	0.71640 (7)	0.12007 (6)	0.59914 (4)	0.0464 (2)	
S4	0.91715 (7)	0.19624 (6)	0.38742 (5)	0.04583 (19)	
F1	0.56368 (19)	0.45268 (16)	0.37042 (15)	0.0697 (6)	
F2	0.4537 (2)	0.3805 (2)	0.46758 (14)	0.0746 (6)	
F3	0.3300 (2)	0.3052 (3)	0.3266 (3)	0.0812 (12)	0.810 (5)
F4	0.4907 (3)	0.3241 (2)	0.25152 (15)	0.0715 (10)	0.810 (5)
F5	0.4988 (3)	0.1142 (3)	0.26891 (18)	0.1259 (13)	
F6	0.4066 (2)	0.1119 (2)	0.3863 (2)	0.1093 (11)	
O1	0.9727 (3)	0.5672 (2)	0.66318 (18)	0.0827 (9)	
O2	0.8080 (3)	−0.3083 (2)	0.4030 (3)	0.0962 (10)	
C1	0.8505 (3)	0.4474 (2)	0.5720 (2)	0.0494 (7)	
C2	0.7748 (3)	0.4263 (2)	0.49994 (19)	0.0442 (6)	
H2	0.7594	0.4784	0.4557	0.053*	
C3	0.7220 (2)	0.3165 (2)	0.49939 (16)	0.0371 (5)	
C4	0.7605 (2)	0.2565 (2)	0.57284 (16)	0.0377 (5)	
C5	0.6309 (2)	0.2760 (2)	0.43218 (15)	0.0356 (5)	
C6	0.5253 (2)	0.3536 (2)	0.40199 (18)	0.0431 (6)	
C7	0.4524 (3)	0.2905 (4)	0.3281 (3)	0.0486 (11)	0.810 (5)
C8	0.4951 (3)	0.1683 (2)	0.3416 (2)	0.0504 (7)	
C9	0.6167 (2)	0.1729 (2)	0.39523 (16)	0.0358 (5)	
C10	0.6979 (2)	0.0740 (2)	0.39929 (16)	0.0364 (5)	
C11	0.8271 (2)	0.0761 (2)	0.39533 (16)	0.0376 (5)	
C12	0.7434 (3)	−0.1179 (2)	0.40298 (19)	0.0461 (6)	
C13	0.6523 (3)	−0.0383 (2)	0.40251 (17)	0.0420 (6)	
H13	0.5682	−0.0557	0.4041	0.050*	
C14	0.9139 (3)	0.5520 (3)	0.5951 (2)	0.0642 (9)	
H14	0.9091	0.6106	0.5552	0.077*	
C15	0.7257 (4)	−0.2395 (3)	0.4026 (2)	0.0620 (9)	
H15	0.6444	−0.2661	0.4020	0.074*	
C16	0.7725 (3)	0.1094 (3)	0.71059 (18)	0.0535 (7)	
H16A	0.8616	0.1157	0.7146	0.080*	
H16B	0.7485	0.0380	0.7334	0.080*	
H16C	0.7373	0.1689	0.7433	0.080*	
C17	1.0583 (3)	0.1414 (3)	0.3464 (2)	0.0593 (8)	
H17A	1.1026	0.0985	0.3908	0.089*	
H17B	1.1095	0.2026	0.3292	0.089*	
H17C	1.0380	0.0939	0.2975	0.089*	

F3'	0.3375 (10)	0.2469 (12)	0.4024 (8)	0.081 (4)	0.190 (5)
F4'	0.3867 (17)	0.3304 (12)	0.2800 (9)	0.090 (5)	0.190 (5)
C7'	0.4250 (7)	0.2804 (7)	0.3523 (7)	0.050 (6)	0.190 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0604 (5)	0.0470 (4)	0.0453 (4)	−0.0169 (3)	−0.0169 (3)	−0.0005 (3)
S2	0.0508 (4)	0.0352 (4)	0.0612 (5)	0.0014 (3)	−0.0004 (3)	0.0031 (3)
S3	0.0593 (4)	0.0397 (4)	0.0387 (3)	−0.0147 (3)	−0.0086 (3)	0.0039 (3)
S4	0.0410 (4)	0.0356 (3)	0.0608 (4)	−0.0068 (3)	0.0023 (3)	−0.0021 (3)
F1	0.0693 (12)	0.0492 (10)	0.0876 (14)	−0.0059 (9)	−0.0189 (10)	0.0269 (10)
F2	0.0707 (13)	0.0872 (16)	0.0671 (12)	0.0286 (11)	0.0134 (10)	−0.0040 (11)
F3	0.0335 (13)	0.0724 (19)	0.134 (3)	0.0019 (12)	−0.0234 (15)	−0.0018 (19)
F4	0.086 (2)	0.0789 (18)	0.0469 (13)	−0.0162 (15)	−0.0187 (12)	0.0168 (12)
F5	0.129 (2)	0.140 (2)	0.0991 (19)	0.062 (2)	−0.0753 (17)	−0.0722 (19)
F6	0.0586 (13)	0.0851 (17)	0.180 (3)	−0.0356 (12)	−0.0303 (16)	0.0536 (18)
O1	0.100 (2)	0.0659 (16)	0.0777 (17)	−0.0379 (15)	−0.0308 (15)	−0.0051 (13)
O2	0.102 (2)	0.0389 (13)	0.147 (3)	0.0066 (14)	0.004 (2)	0.0123 (16)
C1	0.0559 (17)	0.0376 (14)	0.0532 (16)	−0.0134 (12)	−0.0079 (13)	−0.0022 (12)
C2	0.0512 (16)	0.0328 (13)	0.0474 (15)	−0.0053 (11)	−0.0067 (12)	0.0013 (11)
C3	0.0411 (13)	0.0315 (12)	0.0381 (12)	−0.0041 (10)	−0.0035 (10)	−0.0036 (10)
C4	0.0403 (13)	0.0349 (12)	0.0375 (12)	−0.0070 (10)	−0.0034 (10)	−0.0034 (10)
C5	0.0357 (12)	0.0345 (12)	0.0361 (12)	−0.0035 (10)	−0.0019 (9)	0.0020 (10)
C6	0.0421 (14)	0.0399 (14)	0.0469 (15)	0.0008 (11)	−0.0008 (11)	0.0027 (11)
C7	0.0330 (18)	0.057 (2)	0.054 (3)	−0.0033 (17)	−0.007 (2)	0.0045 (19)
C8	0.0456 (16)	0.0448 (15)	0.0584 (17)	−0.0084 (12)	−0.0162 (13)	−0.0051 (13)
C9	0.0360 (12)	0.0358 (12)	0.0350 (12)	−0.0067 (10)	−0.0037 (9)	0.0002 (10)
C10	0.0432 (14)	0.0316 (12)	0.0334 (12)	−0.0063 (10)	−0.0047 (10)	−0.0013 (9)
C11	0.0428 (14)	0.0331 (12)	0.0364 (12)	−0.0040 (10)	−0.0038 (10)	−0.0006 (10)
C12	0.0565 (17)	0.0343 (13)	0.0468 (15)	−0.0083 (12)	−0.0022 (12)	0.0022 (11)
C13	0.0467 (15)	0.0362 (13)	0.0424 (14)	−0.0100 (11)	−0.0044 (11)	−0.0010 (11)
C14	0.076 (2)	0.0452 (17)	0.069 (2)	−0.0222 (16)	−0.0169 (17)	−0.0023 (15)
C15	0.080 (2)	0.0343 (15)	0.070 (2)	−0.0059 (15)	−0.0033 (17)	0.0079 (14)
C16	0.0669 (19)	0.0532 (17)	0.0394 (14)	−0.0042 (15)	−0.0055 (13)	0.0047 (13)
C17	0.0416 (16)	0.0531 (18)	0.084 (2)	−0.0022 (13)	0.0075 (15)	0.0001 (16)
F3'	0.048 (5)	0.102 (8)	0.093 (8)	−0.017 (5)	0.007 (5)	−0.019 (6)
F4'	0.083 (9)	0.094 (8)	0.086 (7)	0.014 (7)	−0.043 (7)	0.001 (6)
C7'	0.057 (10)	0.053 (8)	0.038 (8)	−0.001 (7)	−0.002 (7)	0.014 (6)

Geometric parameters (Å, °)

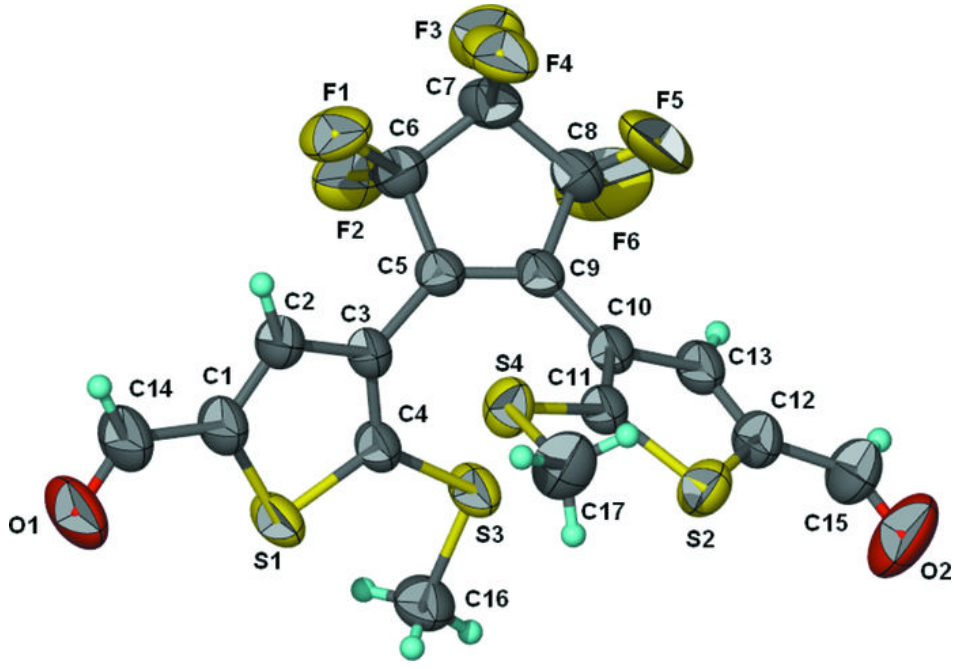
S1—C4	1.722 (2)	C5—C6	1.516 (4)
S1—C1	1.728 (3)	C6—C7	1.543 (4)
S2—C11	1.728 (3)	C6—C7'	1.554 (8)
S2—C12	1.734 (3)	C7—C8	1.534 (5)
S3—C4	1.744 (3)	C8—C9	1.509 (4)
S3—C16	1.799 (3)	C8—C7'	1.545 (8)
S4—C11	1.734 (3)	C9—C10	1.463 (4)

S4—C17	1.803 (3)	C10—C11	1.397 (4)
F1—C6	1.349 (3)	C10—C13	1.424 (3)
F2—C6	1.349 (3)	C12—C13	1.362 (4)
F3—C7	1.329 (4)	C12—C15	1.456 (4)
F4—C7	1.339 (5)	C13—H13	0.9300
F5—C8	1.298 (4)	C14—H14	0.9300
F6—C8	1.384 (4)	C15—H15	0.9300
O1—C14	1.211 (4)	C16—H16A	0.9600
O2—C15	1.205 (4)	C16—H16B	0.9600
C1—C2	1.364 (4)	C16—H16C	0.9600
C1—C14	1.453 (4)	C17—H17A	0.9600
C2—C3	1.423 (3)	C17—H17B	0.9600
C2—H2	0.9300	C17—H17C	0.9600
C3—C4	1.385 (4)	F3'—C7'	1.317 (8)
C3—C5	1.468 (3)	F4'—C7'	1.313 (8)
C5—C9	1.356 (3)		
C4—S1—C1	91.26 (13)	F6—C8—C7'	90.5 (5)
C11—S2—C12	91.55 (13)	C9—C8—C7'	108.8 (3)
C4—S3—C16	102.05 (14)	C5—C9—C10	130.9 (2)
C11—S4—C17	102.34 (14)	C5—C9—C8	109.7 (2)
C2—C1—C14	127.4 (3)	C10—C9—C8	119.3 (2)
C2—C1—S1	112.0 (2)	C11—C10—C13	111.4 (2)
C14—C1—S1	120.6 (2)	C11—C10—C9	125.3 (2)
C1—C2—C3	113.1 (2)	C13—C10—C9	123.3 (2)
C1—C2—H2	123.5	C10—C11—S2	111.69 (19)
C3—C2—H2	123.5	C10—C11—S4	125.5 (2)
C4—C3—C2	111.5 (2)	S2—C11—S4	122.82 (16)
C4—C3—C5	124.7 (2)	C13—C12—C15	126.5 (3)
C2—C3—C5	123.7 (2)	C13—C12—S2	111.7 (2)
C3—C4—S1	112.20 (19)	C15—C12—S2	121.8 (3)
C3—C4—S3	126.69 (19)	C12—C13—C10	113.7 (2)
S1—C4—S3	121.10 (15)	C12—C13—H13	123.2
C9—C5—C3	130.4 (2)	C10—C13—H13	123.2
C9—C5—C6	110.8 (2)	O1—C14—C1	123.8 (3)
C3—C5—C6	118.5 (2)	O1—C14—H14	118.1
F1—C6—F2	105.5 (2)	C1—C14—H14	118.1
F1—C6—C5	113.7 (2)	O2—C15—C12	125.2 (4)
F2—C6—C5	111.3 (2)	O2—C15—H15	117.4
F1—C6—C7	107.9 (3)	C12—C15—H15	117.4
F2—C6—C7	112.7 (3)	S3—C16—H16A	109.5
C5—C6—C7	105.8 (2)	S3—C16—H16B	109.5
F1—C6—C7'	121.9 (4)	H16A—C16—H16B	109.5
F2—C6—C7'	95.4 (4)	S3—C16—H16C	109.5
C5—C6—C7'	107.4 (3)	H16A—C16—H16C	109.5
F3—C7—F4	107.7 (3)	H16B—C16—H16C	109.5
F3—C7—C8	114.6 (3)	S4—C17—H17A	109.5
F4—C7—C8	107.3 (3)	S4—C17—H17B	109.5
F3—C7—C6	114.1 (4)	H17A—C17—H17B	109.5
F4—C7—C6	110.1 (3)	S4—C17—H17C	109.5

C8—C7—C6	102.9 (2)	H17A—C17—H17C	109.5
F5—C8—F6	104.6 (3)	H17B—C17—H17C	109.5
F5—C8—C9	115.2 (3)	F4'—C7'—F3'	116.1 (12)
F6—C8—C9	110.0 (2)	F4'—C7'—C8	115.4 (10)
F5—C8—C7	112.0 (3)	F3'—C7'—C8	100.0 (8)
F6—C8—C7	108.5 (3)	F4'—C7'—C6	110.0 (9)
C9—C8—C7	106.5 (2)	F3'—C7'—C6	112.1 (8)
F5—C8—C7'	124.0 (4)	C8—C7'—C6	101.9 (4)
C4—S1—C1—C2	0.1 (3)	F5—C8—C9—C5	140.8 (3)
C4—S1—C1—C14	177.1 (3)	F6—C8—C9—C5	−101.3 (3)
C14—C1—C2—C3	−176.8 (3)	C7—C8—C9—C5	16.0 (4)
S1—C1—C2—C3	0.0 (4)	C7'—C8—C9—C5	−3.7 (5)
C1—C2—C3—C4	−0.1 (4)	F5—C8—C9—C10	−38.5 (4)
C1—C2—C3—C5	175.6 (3)	F6—C8—C9—C10	79.4 (3)
C2—C3—C4—S1	0.1 (3)	C7—C8—C9—C10	−163.3 (3)
C5—C3—C4—S1	−175.5 (2)	C7'—C8—C9—C10	177.0 (5)
C2—C3—C4—S3	178.9 (2)	C5—C9—C10—C11	−41.3 (4)
C5—C3—C4—S3	3.2 (4)	C8—C9—C10—C11	137.8 (3)
C1—S1—C4—C3	−0.1 (2)	C5—C9—C10—C13	142.7 (3)
C1—S1—C4—S3	−178.93 (19)	C8—C9—C10—C13	−38.2 (4)
C16—S3—C4—C3	−167.9 (3)	C13—C10—C11—S2	−1.5 (3)
C16—S3—C4—S1	10.8 (2)	C9—C10—C11—S2	−177.9 (2)
C4—C3—C5—C9	−41.9 (4)	C13—C10—C11—S4	178.00 (19)
C2—C3—C5—C9	142.9 (3)	C9—C10—C11—S4	1.6 (4)
C4—C3—C5—C6	131.4 (3)	C12—S2—C11—C10	1.0 (2)
C2—C3—C5—C6	−43.8 (4)	C12—S2—C11—S4	−178.51 (18)
C9—C5—C6—F1	−127.5 (3)	C17—S4—C11—C10	−160.0 (2)
C3—C5—C6—F1	58.0 (3)	C17—S4—C11—S2	19.5 (2)
C9—C5—C6—F2	113.5 (3)	C11—S2—C12—C13	−0.3 (2)
C3—C5—C6—F2	−61.0 (3)	C11—S2—C12—C15	176.7 (3)
C9—C5—C6—C7	−9.2 (3)	C15—C12—C13—C10	−177.4 (3)
C3—C5—C6—C7	176.3 (3)	S2—C12—C13—C10	−0.6 (3)
C9—C5—C6—C7'	10.3 (5)	C11—C10—C13—C12	1.4 (3)
C3—C5—C6—C7'	−164.2 (5)	C9—C10—C13—C12	177.8 (2)
F1—C6—C7—F3	−95.2 (4)	C2—C1—C14—O1	174.5 (4)
F2—C6—C7—F3	20.9 (5)	S1—C1—C14—O1	−2.0 (6)
C5—C6—C7—F3	142.8 (3)	C13—C12—C15—O2	180.0 (4)
C7'—C6—C7—F3	45.2 (10)	S2—C12—C15—O2	3.4 (5)
F1—C6—C7—F4	25.9 (4)	F5—C8—C7'—F4'	−12.0 (12)
F2—C6—C7—F4	142.0 (3)	F6—C8—C7'—F4'	−120.0 (10)
C5—C6—C7—F4	−96.1 (3)	C9—C8—C7'—F4'	128.6 (10)
C7'—C6—C7—F4	166.3 (11)	C7—C8—C7'—F4'	42.7 (11)
F1—C6—C7—C8	140.1 (3)	F5—C8—C7'—F3'	113.4 (7)
F2—C6—C7—C8	−103.8 (3)	F6—C8—C7'—F3'	5.4 (7)
C5—C6—C7—C8	18.0 (3)	C9—C8—C7'—F3'	−106.0 (7)
C7'—C6—C7—C8	−79.5 (10)	C7—C8—C7'—F3'	168.0 (14)
F3—C7—C8—F5	88.4 (5)	F5—C8—C7'—C6	−131.2 (5)
F4—C7—C8—F5	−31.1 (4)	F6—C8—C7'—C6	120.7 (5)
C6—C7—C8—F5	−147.2 (3)	C9—C8—C7'—C6	9.3 (7)

F3—C7—C8—F6	−26.5 (5)	C7—C8—C7'—C6	−76.6 (10)
F4—C7—C8—F6	−146.0 (3)	F1—C6—C7'—F4'	−0.8 (12)
C6—C7—C8—F6	97.9 (3)	F2—C6—C7'—F4'	111.2 (10)
F3—C7—C8—C9	−144.9 (4)	C5—C6—C7'—F4'	−134.5 (10)
F4—C7—C8—C9	95.6 (3)	C7—C6—C7'—F4'	−46.4 (12)
C6—C7—C8—C9	−20.5 (4)	F1—C6—C7'—F3'	−131.7 (8)
F3—C7—C8—C7'	−44.8 (10)	F2—C6—C7'—F3'	−19.7 (9)
F4—C7—C8—C7'	−164.3 (11)	C5—C6—C7'—F3'	94.7 (9)
C6—C7—C8—C7'	79.6 (10)	C7—C6—C7'—F3'	−177.3 (15)
C3—C5—C9—C10	−11.3 (5)	F1—C6—C7'—C8	122.1 (5)
C6—C5—C9—C10	175.0 (3)	F2—C6—C7'—C8	−125.8 (5)
C3—C5—C9—C8	169.5 (3)	C5—C6—C7'—C8	−11.5 (7)
C6—C5—C9—C8	−4.2 (3)	C7—C6—C7'—C8	76.6 (10)

Fig. 1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