



Crystal structure and Hirshfeld surface analysis of (*E*)-3-(2-chloro-4-fluorophenyl)-1-(2,5-dichlorothiophen-3-yl)prop-2-en-1-one

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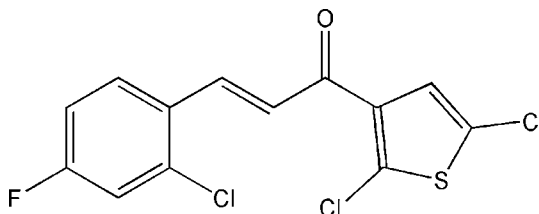
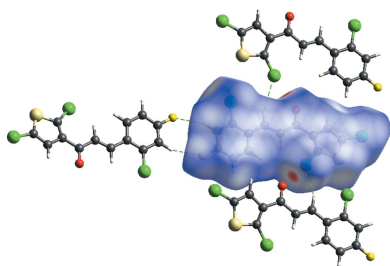
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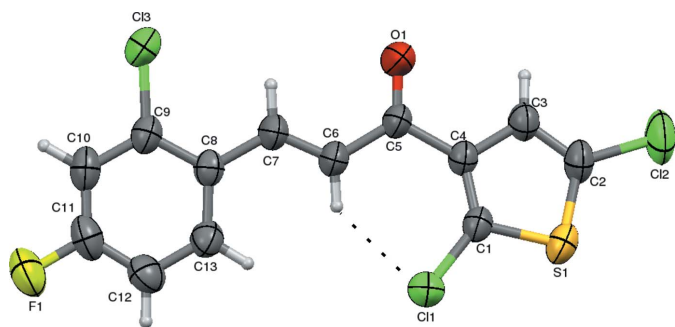
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In the title chalcone–thiophene derivative, $C_{13}H_6Cl_3FOS$, the aromatic rings are inclined to one another by $12.9(2)^\circ$, and the thiophene ring is affected by π -conjugation. In the crystal, molecules are linked by $C-H \cdots F$ hydrogen bonds, forming an $R_2^2(8)$ ring motif. A Hirshfeld surface analysis was conducted to verify the contribution of the different intermolecular interactions. The shape-index surface clearly shows that the two sides of the molecules are involved in the same contacts with neighbouring molecules and the curvedness plots show flat surface patches characteristic of planar stacking.

1. Chemical context

Natural products are important sources in the search for new agents for cancer therapies with minimal side effects. Chalcones, considered to be the precursor of flavonoids and isoflavonoids, are abundant in edible plants. Compounds with the 1,3-diphenylprop-2-en-1-one framework are described by its generic term ‘chalcone’. They consist of open-chain flavonoids in which the two aromatic rings are joined by a three-carbon α,β -unsaturated carbonyl system. These are coloured compounds because of the presence of the $-CO-CH=CH-$ chromophore, which depends in the presence of other auxochromes. Accumulating evidence has shown that chalcones and their derivatives could inhibit tumor initiation and progression. In view of the above, and as a part of our ongoing research on chalcone derivatives (Naveen *et al.*, 2017; Lokeshwari *et al.*, 2017; Tejkiran *et al.*, 2016), we report herein the synthesis, crystal structure and Hirshfeld surface analysis of the title compound.




Figure 1

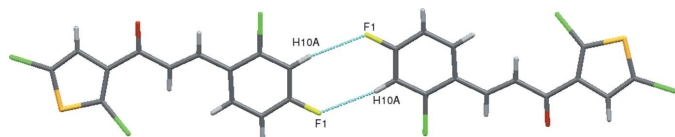
The molecular structure of the title compound, indicating the atom-numbering scheme. The intramolecular C–H···Cl hydrogen bond (dashed line) closes an $S(6)$ motif. Displacement ellipsoids are drawn at the 50% probability level.

2. Structural commentary

The molecular structure of the title compound, shown in Fig. 1, is comprised of two aromatic rings (chlorofluorophenyl and dichlorothiophene) linked by C=C–C(=O)–C enone bridge. The bond lengths and bond angles are normal and the molecular conformation is characterized by a dihedral angle of $12.9(2)^\circ$ between the mean planes of the two aromatic rings. The olefinic double bond C6=C7 of $1.303(6)$ Å is in an E configuration and is Csp^2 hybridized. The unsaturated keto group is in a syn-periplanar conformation with respect to the olefinic double bond, which is evident from the torsion angle value of $-0.5(8)^\circ$ for the atoms O1–C5–C6–C7. The thiophene ring is affected by π conjugation. This can be explained by the longer C=S values of $1.703(6)$ and $1.714(4)$ Å for S1=C2 and S1=C1, respectively. The bond-angle values O1–C5–C6 [$121.9(4)^\circ$], O1–C5–C4 [$118.2(4)^\circ$] and C5–C6–C7 = $125.14(4)^\circ$ about C5 indicate that the carbon atom is in a distorted trigonal-planar configuration, which is due to steric hindrance of the oxygen atom. The molecular structure is stabilized by an intramolecular C6–H6A···Cl1 hydrogen bond (Table 1) that closes an $S(6)$ motif, as shown in Fig. 1.

3. Supramolecular features

In the crystal, the molecules are linked by C–H···F hydrogen bonds, forming an $R_2^2(8)$ ring motif as shown in Fig. 2. The structure also features π – π interactions: Cg1···Cg1($x-1, y, z$) = $3.956(3)$ Å [$\alpha = 0^\circ, \beta = 24.0^\circ, \gamma = 24.0^\circ$, perpendicular distance of Cg1 on itself = $3.6131(19)$ Å] and Cg2···Cg2($x+1, y, z$) = $3.957(3)$ Å [$\alpha = 0^\circ, \beta = 27.3^\circ, \gamma = 27.3^\circ$] where Cg1 and


Figure 2

The $R_2^2(8)$ ring motif.

Table 1

Hydrogen-bond geometry (Å, $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C6–H6A···Cl1	0.93	2.47	3.207 (5)	136
C10–H10A···F1 ⁱ	0.93	2.54	3.433 (6)	160

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

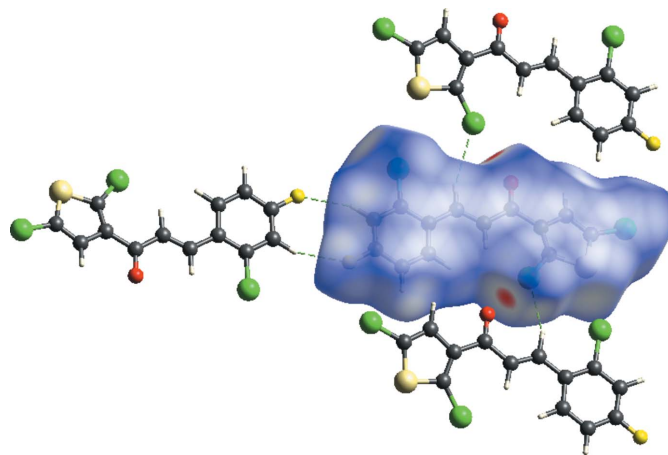
Cg2 are the centroids of the S1/C1–C4 and C8–C13 rings, respectively.

4. Database survey

A survey of the Cambridge Structural Database (CSD, Version 5.39, last update November 2016; Groom *et al.*, 2016) using (E)-3-(phenyl)-1-(2,5-dichlorothiophen-3-yl)prop-2-en-1-one as the main skeleton revealed the presence of three structures containing a similar 2,5-dichlorothiophene–chalcone moiety to the title compound but with different substituents on the terminal phenyl rings, *viz.* [(E)-1-(2,5-dichloro-3-thienyl)-3-(X)prop-2-en-1-one], where $X = 4$ -(dimethylamino)phenyl (Dutkiewicz *et al.*, 2010), 3,4-dimethoxyphenyl (Harrison *et al.*, 2010*a*) and 6-methoxy-2-naphthyl (Jasinski *et al.*, 2010). In these three compounds, the dihedral angles between the central and terminal phenyl/naphthyl ring are in the range 2.13 – 11.90° . The difference may arise from the intermolecular hydrogen bonds between adjacent molecules.

5. Hirshfeld surface analysis

Hirshfeld surfaces and fingerprint plots were generated for the title compound based on the crystallographic information file (CIF) using *CrystalExplorer* (McKinnon *et al.*, 2007). Hirshfeld surfaces enable the visualization of intermolecular interactions with different colours and colour intensity representing short or long contacts and indicating the relative strength of the interactions. Figs. 3 and 4 show the Hirshfeld


Figure 3

View of the three-dimensional Hirshfeld surface of the title compound mapped over d_{norm} .

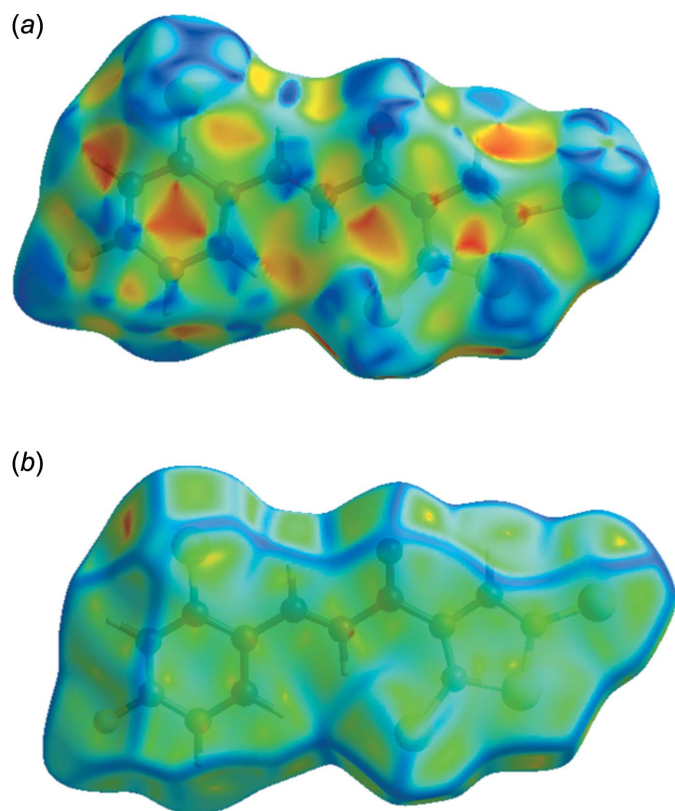


Figure 4
Hirshfeld surface of the title compound mapped over (a) shape-index and (b) curvedness.

surfaces mapped over d_{norm} (−0.139 to 1.120 a.u.) and shape-index (−1.0 to 1.0 a.u.), respectively. The calculated volume inside the Hirshfeld surface is 325.37 Å³ in the area of 310.17 Å².

In Fig. 4, the dark spots near atoms Cl1 and F1 result from the C6—H6A···Cl1 and C10—H10A···F1 interactions, which play a significant role in the molecular packing of the title compound. The Hirshfeld surfaces illustrated in Fig. 4 also reflect the involvement of different atoms in the intermolecular interactions through the appearance of blue and red regions around the participating atoms, which correspond to positive and negative electrostatic potential, respectively. The shape-index surface clearly shows that the two sides of the molecules are involved in the same contacts with neighbouring molecules while the curvedness plots show flat surface patches characteristic of planar stacking.

The overall two-dimensional fingerprint plot for the title compound and those delineated into Cl···H/H···Cl, C···C, Cl···Cl, Cl···S/S···Cl, H···H, F···H/H···F, C···H/H···C contacts are illustrated in Fig. 5; the percentage contributions from the different interatomic contacts to the Hirshfeld surfaces are as follows: Cl···H (13.8%), C···C (12.7%), Cl···Cl (12.4%), Cl···S (10.7%), F···H (10.2%), H···H (10.1%), C···H (8.3%). The percentage contributions for other intermolecular contacts are less than 5% in the Hirshfeld surface mapping.

6. Synthesis and crystallization

The title compound was synthesized as per the procedure reported earlier (Kumar *et al.*, 2013a,b; Chidan Kumar *et al.*, 2014). 1-(2,5-Dichlorothiophen-3-yl)ethanone (0.01 mol) (Harrison *et al.*, 2010b) and 2,4-dichlorobenzaldehyde (0.01 mol) were dissolved in 20 ml of methanol. A catalytic amount of NaOH was added to the solution dropwise with vigorous stirring. The reaction mixture was stirred for about 2 h at room temperature. The formed crude products were filtered off, washed successively with distilled water and

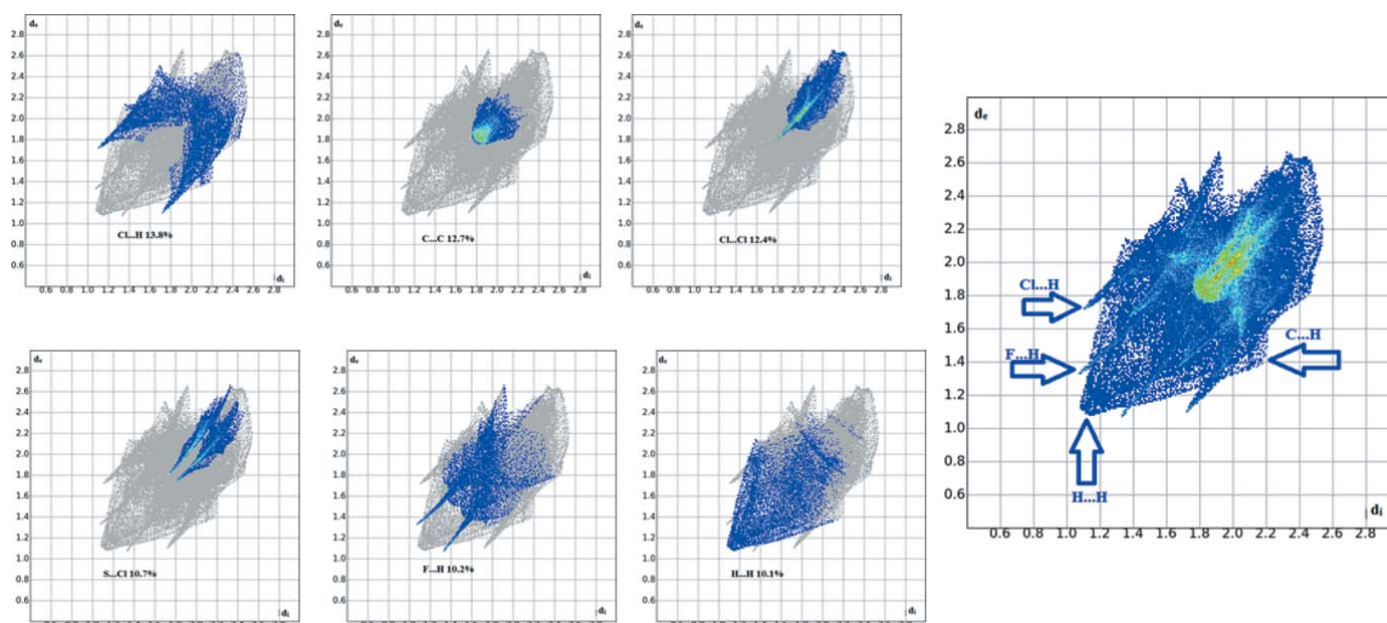


Figure 5
Two-dimensional fingerprint plots showing the percentage contributions of the various interactions.

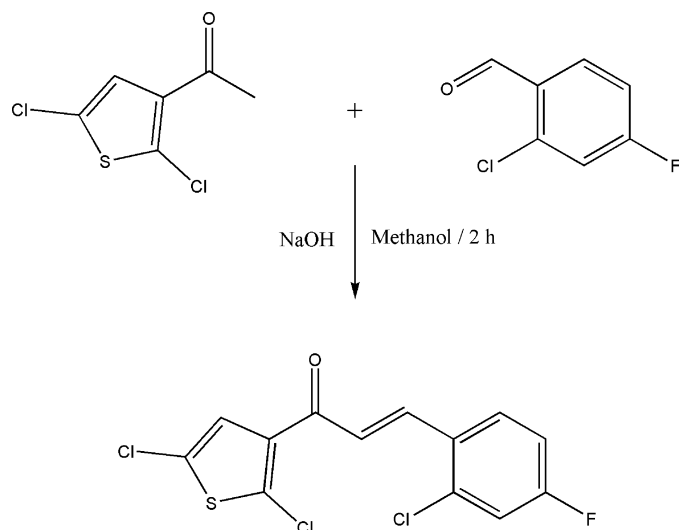


Figure 6
Synthesis of the title compound.

recrystallized from methanol to give the title chalcone. The reaction scheme is shown in Fig. 6. The melting point (306–309 K) was determined using a Stuart Scientific (UK) apparatus.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. C-bound H atoms were positioned geometrically (C–H = 0.95–0.99 Å) and refined using a riding model with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Acknowledgements

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Table 2

Experimental details.

Crystal data	
Chemical formula	C ₁₃ H ₆ Cl ₃ FOS
<i>M_r</i>	335.60
Crystal system, space group	Monoclinic, <i>P</i> ₂ ₁ / <i>c</i>
Temperature (K)	294
<i>a</i> , <i>b</i> , <i>c</i> (Å)	3.9564 (8), 13.367 (2), 25.173 (5)
β (°)	93.363 (4)
<i>V</i> (Å ³)	1329.0 (4)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.84
Crystal size (mm)	0.44 × 0.19 × 0.14
Data collection	
Diffractometer	Bruker APEXII DUO CCD area-detector
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2012)
<i>T</i> _{min} – <i>T</i> _{max}	0.708, 0.894
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	3901, 3901, 2430
<i>R</i> _{int}	0.000
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.707
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.076, 0.218, 1.04
No. of reflections	3901
No. of parameters	173
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.46, –0.48

Computer programs: *APEX2* and *SAINT* (Bruker, 2012), *SHELXS97* (Sheldrick, 2008), *SHELXL2013* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2006) and *PLATON* (Spek, 2009).

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Computing details

Data collection: *APEX2* (Bruker, 2012); cell refinement: *SAINT* (Bruker, 2012); data reduction: *SAINT* (Bruker, 2012); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2015); molecular graphics: *SHELXL2013* (Sheldrick, 2015) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL2013* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

(*E*)-3-(2-Chloro-4-fluorophenyl)-1-(2,5-dichlorothiophen-3-yl)prop-2-en-1-one

Crystal data

C₁₃H₆Cl₃FOS

M_r = 335.60

Monoclinic, *P*2₁/*c*

Hall symbol: -P 2ybc

a = 3.9564 (8) Å

b = 13.367 (2) Å

c = 25.173 (5) Å

β = 93.363 (4)°

V = 1329.0 (4) Å³

Z = 4

F(000) = 672

D_x = 1.677 Mg m⁻³

Mo *Kα* radiation, λ = 0.71073 Å

Cell parameters from 2430 reflections

θ = 1.6–30.2°

μ = 0.84 mm⁻¹

T = 294 K

Rectangle, green

0.44 × 0.19 × 0.14 mm

Data collection

Bruker APEXII DUO CCD area-detector diffractometer

Radiation source: Rotating Anode

Graphite monochromator

Detector resolution: 18.4 pixels mm⁻¹

φ and ω scans

Absorption correction: multi-scan (SADABS; Bruker, 2012)

T_{min} = 0.708, *T_{max}* = 0.894

3901 measured reflections

3901 independent reflections

2430 reflections with *I* > 2σ(*I*)

R_{int} = 0.0000

θ_{max} = 30.2°, θ_{min} = 1.6°

h = -5→5

k = -18→18

l = -2→35

Refinement

Refinement on *F*²

Least-squares matrix: full

R [*F*² > 2σ(*F*²)] = 0.076

wR (*F*²) = 0.218

S = 1.04

3901 reflections

173 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
 $w = 1/[\sigma^2(F_o^2) + (0.0673P)^2 + 2.8657P]$
 where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.46 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.48 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs 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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	0.3576 (4)	0.89705 (9)	0.29850 (5)	0.0644 (5)
C12	0.2067 (5)	1.14124 (14)	0.48102 (5)	0.0892 (6)
C13	1.1255 (5)	1.22982 (11)	0.10663 (6)	0.0863 (6)
S1	0.2273 (3)	0.97600 (10)	0.40296 (5)	0.0581 (4)
F1	1.3011 (10)	0.8888 (3)	0.03284 (14)	0.0890 (16)
O1	0.6247 (13)	1.2332 (3)	0.28547 (15)	0.0826 (16)
C1	0.3669 (11)	0.9974 (3)	0.34077 (16)	0.0452 (11)
C2	0.2951 (13)	1.0983 (4)	0.41922 (17)	0.0576 (15)
C3	0.4177 (12)	1.1522 (4)	0.37994 (16)	0.0518 (16)
C4	0.4643 (11)	1.0936 (3)	0.33320 (15)	0.0438 (11)
C5	0.6036 (13)	1.1423 (3)	0.28592 (16)	0.0503 (14)
C6	0.7148 (13)	1.0813 (3)	0.24247 (17)	0.0528 (14)
C7	0.8427 (14)	1.1157 (4)	0.19955 (16)	0.0553 (14)
C8	0.9626 (11)	1.0570 (3)	0.15588 (15)	0.0446 (11)
C9	1.0932 (12)	1.1014 (4)	0.11131 (17)	0.0505 (16)
C10	1.2095 (12)	1.0457 (4)	0.06983 (17)	0.0567 (16)
C11	1.1865 (13)	0.9448 (4)	0.0731 (2)	0.0621 (19)
C12	1.0579 (14)	0.8963 (4)	0.1151 (2)	0.0633 (17)
C13	0.9467 (13)	0.9528 (4)	0.15625 (18)	0.0535 (16)
H3A	0.46730	1.22000	0.38260	0.0620*
H6A	0.69310	1.01230	0.24550	0.0630*
H7A	0.85890	1.18480	0.19660	0.0660*
H10A	1.30020	1.07640	0.04070	0.0680*
H12A	1.04550	0.82680	0.11580	0.0760*
H13A	0.85860	0.92070	0.18510	0.0640*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0855 (10)	0.0491 (6)	0.0602 (7)	-0.0030 (6)	0.0169 (6)	-0.0015 (5)
C12	0.1049 (13)	0.1212 (13)	0.0442 (6)	-0.0094 (11)	0.0269 (7)	-0.0147 (7)
C13	0.1298 (15)	0.0642 (8)	0.0694 (8)	-0.0049 (9)	0.0430 (9)	0.0128 (6)

S1	0.0607 (8)	0.0698 (8)	0.0448 (6)	-0.0031 (6)	0.0114 (5)	0.0138 (5)
F1	0.098 (3)	0.096 (3)	0.076 (2)	0.013 (2)	0.030 (2)	-0.0231 (18)
O1	0.141 (4)	0.0503 (19)	0.060 (2)	-0.011 (2)	0.037 (2)	-0.0004 (16)
C1	0.043 (2)	0.054 (2)	0.0392 (18)	0.0025 (19)	0.0072 (16)	0.0064 (16)
C2	0.059 (3)	0.078 (3)	0.0365 (19)	-0.005 (3)	0.0095 (19)	-0.004 (2)
C3	0.056 (3)	0.060 (3)	0.040 (2)	-0.003 (2)	0.0078 (19)	-0.0031 (18)
C4	0.045 (2)	0.051 (2)	0.0357 (18)	-0.0023 (19)	0.0060 (16)	0.0001 (16)
C5	0.066 (3)	0.048 (2)	0.0378 (19)	-0.004 (2)	0.0118 (19)	0.0039 (17)
C6	0.067 (3)	0.051 (2)	0.042 (2)	0.000 (2)	0.017 (2)	0.0039 (18)
C7	0.076 (3)	0.052 (2)	0.039 (2)	0.000 (2)	0.013 (2)	0.0023 (17)
C8	0.041 (2)	0.056 (2)	0.0367 (18)	0.0005 (19)	0.0016 (16)	0.0010 (16)
C9	0.050 (3)	0.061 (3)	0.041 (2)	0.000 (2)	0.0061 (18)	0.0071 (18)
C10	0.050 (3)	0.081 (3)	0.040 (2)	0.002 (3)	0.0093 (19)	0.001 (2)
C11	0.052 (3)	0.081 (4)	0.054 (3)	0.009 (3)	0.010 (2)	-0.015 (2)
C12	0.061 (3)	0.059 (3)	0.071 (3)	0.010 (3)	0.013 (3)	-0.006 (2)
C13	0.057 (3)	0.057 (3)	0.047 (2)	0.006 (2)	0.008 (2)	0.0071 (19)

Geometric parameters (Å, °)

C11—C1	1.711 (4)	C7—C8	1.453 (6)
C12—C2	1.713 (5)	C8—C9	1.395 (6)
C13—C9	1.726 (6)	C8—C13	1.394 (7)
S1—C1	1.714 (4)	C9—C10	1.383 (7)
S1—C2	1.703 (5)	C10—C11	1.355 (8)
F1—C11	1.359 (6)	C11—C12	1.364 (7)
O1—C5	1.218 (6)	C12—C13	1.375 (7)
C1—C4	1.359 (6)	C3—H3A	0.9300
C2—C3	1.337 (7)	C6—H6A	0.9300
C3—C4	1.434 (6)	C7—H7A	0.9300
C4—C5	1.490 (6)	C10—H10A	0.9300
C5—C6	1.453 (6)	C12—H12A	0.9300
C6—C7	1.303 (6)	C13—H13A	0.9300
C1—S1—C2	90.3 (2)	C13—C9—C10	117.0 (4)
C11—C1—S1	116.2 (2)	C8—C9—C10	122.2 (5)
C11—C1—C4	130.6 (3)	C9—C10—C11	117.6 (4)
S1—C1—C4	113.3 (3)	F1—C11—C10	118.5 (4)
C12—C2—S1	120.2 (3)	F1—C11—C12	118.2 (5)
C12—C2—C3	126.4 (4)	C10—C11—C12	123.4 (5)
S1—C2—C3	113.5 (4)	C11—C12—C13	118.3 (5)
C2—C3—C4	112.5 (5)	C8—C13—C12	121.8 (4)
C1—C4—C3	110.5 (4)	C2—C3—H3A	124.00
C1—C4—C5	130.3 (4)	C4—C3—H3A	124.00
C3—C4—C5	119.2 (4)	C5—C6—H6A	117.00
O1—C5—C4	118.2 (4)	C7—C6—H6A	117.00
O1—C5—C6	121.9 (4)	C6—C7—H7A	117.00
C4—C5—C6	119.9 (4)	C8—C7—H7A	117.00
C5—C6—C7	125.1 (4)	C9—C10—H10A	121.00

C6—C7—C8	126.6 (5)	C11—C10—H10A	121.00
C7—C8—C9	122.1 (4)	C11—C12—H12A	121.00
C7—C8—C13	121.2 (4)	C13—C12—H12A	121.00
C9—C8—C13	116.7 (4)	C8—C13—H13A	119.00
C13—C9—C8	120.7 (4)	C12—C13—H13A	119.00
C2—S1—C1—C11	-178.6 (3)	C4—C5—C6—C7	-179.4 (5)
C2—S1—C1—C4	0.7 (4)	C5—C6—C7—C8	178.7 (5)
C1—S1—C2—C12	179.7 (3)	C6—C7—C8—C9	179.5 (5)
C1—S1—C2—C3	-0.3 (4)	C6—C7—C8—C13	0.6 (8)
C11—C1—C4—C3	178.2 (4)	C7—C8—C9—C13	1.2 (6)
C11—C1—C4—C5	-1.8 (8)	C7—C8—C9—C10	179.6 (5)
S1—C1—C4—C3	-0.9 (5)	C13—C8—C9—C13	-179.9 (4)
S1—C1—C4—C5	179.0 (4)	C13—C8—C9—C10	-1.5 (7)
C12—C2—C3—C4	179.8 (4)	C7—C8—C13—C12	179.7 (5)
S1—C2—C3—C4	-0.2 (6)	C9—C8—C13—C12	0.8 (7)
C2—C3—C4—C1	0.7 (6)	C13—C9—C10—C11	179.8 (4)
C2—C3—C4—C5	-179.2 (4)	C8—C9—C10—C11	1.4 (7)
C1—C4—C5—O1	169.0 (5)	C9—C10—C11—F1	-179.7 (4)
C1—C4—C5—C6	-12.0 (8)	C9—C10—C11—C12	-0.5 (8)
C3—C4—C5—O1	-11.1 (7)	F1—C11—C12—C13	179.0 (5)
C3—C4—C5—C6	167.9 (4)	C10—C11—C12—C13	-0.2 (8)
O1—C5—C6—C7	-0.5 (8)	C11—C12—C13—C8	0.0 (8)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C6—H6 <i>A</i> ...C11	0.93	2.47	3.207 (5)	136
C10—H10 <i>A</i> ...F1 ⁱ	0.93	2.54	3.433 (6)	160

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