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4,4′-Bis(4-fluorophenylsulfonyl)oxydibenzene

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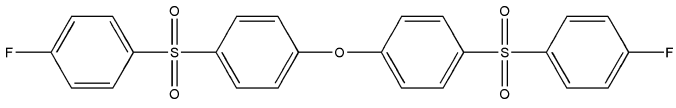
Key indicators: single-crystal X-ray study; T = 180 K; mean σ(C–C) = 0.004 Å; R factor = 0.039; wR factor = 0.096; data-to-parameter ratio = 9.2.

In the title compound, $C_{24}H_{16}F_2O_5S_2$, the benzene rings of the central oxydibenzene unit are inclined at an angle of 83.49 (8)° to one another. Each of these benzene rings carries a *p*-substituted 4-fluorosulfonylbenzene group with dihedral angles of 77.27 (8) and 62.06 (11)° between the respective 4-fluorosulfonylbenzene and oxydibenzene rings. In the crystal structure, a complex network of C—H···F and C—H···O hydrogen bonds and a C—H···π interaction link the molecules into columns along the *bc* diagonal.

Related literature

For details of structure–property relationships of crystalline polysulfones, see Carlier *et al.* (1992), and for information on structure determinations of polymers from powder data, see Colquhoun *et al.* (2003). For related structures, see for example Colquhoun *et al.* (2005, 2002) and Holman *et al.* (2001).



Experimental

Crystal data

$C_{24}H_{16}F_2O_5S_2$
M_r = 486.49
Monoclinic, $P2_1/c$
a = 14.0437 (6) Å
b = 16.0590 (6) Å
c = 9.6644 (3) Å
β = 102.223 (1)°
V = 2130.18 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.30 mm^{-1}
T = 180 (2) K
0.23 × 0.07 × 0.05 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.954, T_{max} = 0.996
10006 measured reflections
2736 independent reflections
2084 reflections with $I > 2\sigma(I)$
R_{int} = 0.055
θ_{max} = 22.4°

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.096
S = 1.06
2736 reflections
298 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*1 is the centroid of the C1–C6 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2A···O2^{i}	0.95	2.55	3.206 (4)	126
C6—H6A···O5^{ii}	0.95	2.53	3.337 (4)	143
C14—H14A···O2^{iii}	0.95	2.47	3.361 (4)	157
C17—H17A···O4^{iv}	0.95	2.60	3.529 (4)	168
C11—H11A···F1^{v}	0.95	2.67	3.396 (4)	134
C23—H23A···F1^{vi}	0.95	2.65	3.373 (5)	133
C11—H11A···Cg1^{iv}	0.95	2.97	3.541 (3)	120

Symmetry codes: (i) $-x, -y, -z-1$; (ii) $x-1, y, z-1$; (iii) $-x, y+\frac{1}{2}, -z-\frac{1}{2}$; (iv) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (v) $x, y, z+1$; (vi) $x+1, -y+\frac{1}{2}, z+\frac{3}{2}$.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*, *enCIFer* (Allen *et al.*, 2004) and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GW2026).

References

Allen, F. H., Johnson, O., Shields, G. P., Smith, B. R. & Towler, M. (2004). *J. Appl. Cryst.* **37**, 335–338.
Altomare, A., Cascarano, G., Giacovazzo, C. & Guagliardi, A. (1993). *J. Appl. Cryst.* **26**, 343–350.
Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Carlier, V., Devaux, J., Legras, R. & McGrail, P. T. (1992). *Macromolecules*, **25**, 6646–6650.
Colquhoun, H. M., Aldred, P. L., Zhu, Z. & Williams, D. J. (2003). *Macromolecules*, **36**, 6416–6421.
Colquhoun, H. M., Williams, D. J. & Zhu, Z. (2002). *J. Am. Chem. Soc.* **124**, 13346–13347.
Colquhoun, H. M., Zhu, Z., Dudman, C. C., O'Mahoney, C. A., Williams, D. J. & Drew, M. G. B. (2005). *Macromolecules*, **38**, 10413–10420.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Holman, K. T., Martin, S. M., Parker, D. P. & Ward, M. D. (2001). *J. Am. Chem. Soc.* **123**, 4421–4431.
Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

supplementary materials

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4,4'-Bis(4-fluorophenylsulfonyl)oxydibenzene

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Comment

Polysulphones are an important class of high temperature thermoplastics. The properties of these polymers are dependent on the flexibility of the chain (for the glass transition temperature) and any crystallinity (for the melting point transition) (Carlier *et al.*, 1992). An important method of obtaining and refining the *x*-ray structure for any polymer is by using the *x*-ray structure of related oligomers (Colquhoun *et al.*, 2003), thus any information on the packing motifs of extended oligomers is very useful. During the preparation of a polysulfone dendrimer, the title compound was obtained as a minor impurity. It probably arose from the nucleophilic attack of trace amounts of water on 4-fluorophenylsulfone under the reaction conditions (160 °C in DMSO).

The benzene rings of the central oxydibenzene unit are inclined at an angle of 83.49 (8)° to one another. Each of these benzene rings carries a *p*-substituted 4-fluorosulfonylbenzene system with dihedral angles of 77.27 (8)° and 62.06 (11)° between the C1···C6 & C7···C9 and between the C13···C18 & C19···C24 rings respectively.

In the crystal structure, a complex network of C—H···F, C—H···O hydrogen bonds and a C11—H11A···*Cg*1^{vii} π-interaction link the molecules into columns along the *bc* diagonal (*Cg*1 is the centroid of the C1···C6 ring; iv = *x*, −*y* + 1/2, *z* + 1/2), Table 1.

Experimental

To a solution of a generation 1 polysulfone dendrimer (0.50 g, 0.6 mmol) and 4-fluorophenyl sulphone (3.08 g, 12.1 mmol) in anhydrous DMSO (40 ml) was added Na_2CO_3 (0.26 g, 2.4 mmol). The mixture was heated under nitrogen at 160 °C for 5 h, water (60 ml) was added and the mixture extracted with ethyl acetate (3 *x* 40 ml). The combined extracts were then dried over magnesium sulfate, filtered and concentrated *in vacuo*. Column chromatography using 80:20 hexane:ethyl acetate yielded 0.02 g (1%) of a white solid, the title compound (I). Rf (hexane:ethyl acetate 1:1) 0.80; m.p 140–142 °C; IR (KBr) 2900, 1750, 1590, 1505, 1490, 1410, 1300, 1250, 1150, 1010 cm^{-1}; 1H NMR (400 MHz) δ ($CDCl_3$) 7.96–7.88 (m, 4H, H-3, H-6), 7.18 (t, 2H, H-2, ^{3}JHH = 8.5 Hz), 7.08 (d, 2H, H-7, ^{3}JHH = 9.0 Hz). Colourles needles were obtained by layering a solution in ethyl acetate with hexane.

Refinement

The crystals were small and very weakly diffracting so that high angle reflections were not obtained beyond θ(max) = 22.5°. All H-atoms were positioned geometrically and refined using a riding model with d(C—H) = 0.95 Å, U_{iso} = 1.2U_{eq} (C).

Figures

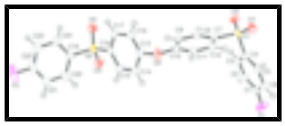

Fig. 1. The structure of (I) showing the atom numbering with ellipsoids drawn at the 50% probability level.

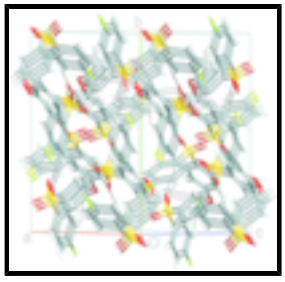

Fig. 2. Crystal packing for (I) with hydrogen bonds drawn as dashed lines.

4,4'-Bis(4-fluorophenylsulfonyl)oxydibenzene

Crystal data

$C_{24}H_{16}F_2O_5S_2$	F_{000} = 1000
M_r = 486.49	D_x = 1.517 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 6093 reflections
a = 14.0437 (6) Å	θ = 1.0–22.5º
b = 16.0590 (6) Å	μ = 0.30 mm^{-1}
c = 9.6644 (3) Å	T = 180 (2) K
β = 102.223 (1)º	Needle, colourless
V = 2130.18 (14) Å^3	0.23 × 0.07 × 0.05 mm
Z = 4	

Data collection

Nonius KappaCCD diffractometer	2736 independent reflections
Radiation source: fine-focus sealed tube	2084 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.055
T = 180(2) K	θ_{max} = 22.4º
Thin–slice ω and φ scans	θ_{min} = 3.5º
Absorption correction: multi-scan (SORTAV; Blessing, 1995)	h = −15→15
T_{min} = 0.954, T_{max} = 0.996	k = −17→16
10006 measured reflections	l = −10→10

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.039$	H-atom parameters constrained
$wR(F^2) = 0.096$	$w = 1/[\sigma^2(F_o^2) + (0.0393P)^2 + 0.9105P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} < 0.001$
2736 reflections	$\Delta\rho_{max} = 0.28$ e Å^{-3}
298 parameters	$\Delta\rho_{min} = -0.34$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. Poorly diffracting crystals (ThetaMax=22.5 degrees).

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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	−0.13021 (6)	0.01325 (5)	−0.26488 (8)	0.0311 (3)
S2	0.48394 (6)	0.32919 (6)	0.15358 (8)	0.0318 (3)
O1	−0.21631 (15)	−0.01428 (14)	−0.2205 (2)	0.0387 (6)
O2	−0.06039 (15)	−0.04715 (13)	−0.2910 (2)	0.0364 (6)
O3	0.06855 (15)	0.26534 (14)	0.1351 (2)	0.0386 (6)
O4	0.48671 (16)	0.35984 (15)	0.0145 (2)	0.0428 (6)
O5	0.53284 (15)	0.25302 (14)	0.2019 (2)	0.0439 (6)
F1	−0.25344 (14)	0.20090 (14)	−0.79030 (19)	0.0568 (6)
F2	0.65833 (17)	0.59150 (16)	0.5413 (2)	0.0847 (8)
C1	−0.2260 (2)	0.1570 (2)	−0.6682 (3)	0.0370 (9)
C2	−0.1336 (2)	0.1256 (2)	−0.6377 (3)	0.0406 (9)
H2A	−0.0907	0.1334	−0.7005	0.049*
C3	−0.1043 (2)	0.0820 (2)	−0.5124 (3)	0.0341 (8)
H3A	−0.0404	0.0596	−0.4879	0.041*
C4	−0.1681 (2)	0.0710 (2)	−0.4232 (3)	0.0285 (8)
C5	−0.2618 (2)	0.1028 (2)	−0.4580 (3)	0.0347 (9)
H5A	−0.3056	0.0944	−0.3967	0.042*
C6	−0.2913 (2)	0.1470 (2)	−0.5834 (3)	0.0394 (9)
H6A	−0.3551	0.1696	−0.6092	0.047*
C7	−0.0686 (2)	0.08542 (19)	−0.1416 (3)	0.0266 (8)
C8	0.0317 (2)	0.0945 (2)	−0.1237 (3)	0.0309 (8)

H8A	0.0670	0.0599	−0.1747	0.037*
C9	0.0800 (2)	0.1539 (2)	−0.0319 (3)	0.0316 (8)
H9A	0.1484	0.1607	−0.0197	0.038*
C10	0.0276 (2)	0.2034 (2)	0.0422 (3)	0.0275 (8)
C11	−0.0724 (2)	0.1941 (2)	0.0261 (3)	0.0306 (8)
H11A	−0.1075	0.2284	0.0780	0.037*
C12	−0.1202 (2)	0.1350 (2)	−0.0651 (3)	0.0314 (8)
H12A	−0.1886	0.1279	−0.0761	0.038*
C13	0.1672 (2)	0.2833 (2)	0.1457 (3)	0.0308 (8)
C14	0.1924 (2)	0.3476 (2)	0.0666 (3)	0.0367 (9)
H14A	0.1435	0.3803	0.0081	0.044*
C15	0.2898 (2)	0.3641 (2)	0.0732 (3)	0.0372 (9)
H15A	0.3083	0.4079	0.0182	0.045*
C16	0.3603 (2)	0.31666 (19)	0.1601 (3)	0.0266 (8)
C17	0.3337 (2)	0.2549 (2)	0.2444 (3)	0.0336 (8)
H17A	0.3823	0.2246	0.3079	0.040*
C18	0.2363 (2)	0.2377 (2)	0.2360 (3)	0.0337 (8)
H18A	0.2173	0.1947	0.2921	0.040*
C19	0.5321 (2)	0.4080 (2)	0.2748 (3)	0.0285 (8)
C20	0.5202 (2)	0.4902 (2)	0.2328 (3)	0.0392 (9)
H20A	0.4836	0.5037	0.1412	0.047*
C21	0.5614 (3)	0.5524 (2)	0.3236 (4)	0.0483 (10)
H21A	0.5527	0.6093	0.2969	0.058*
C22	0.6147 (3)	0.5304 (3)	0.4519 (4)	0.0495 (11)
C23	0.6269 (2)	0.4498 (3)	0.4990 (4)	0.0481 (10)
H23A	0.6635	0.4372	0.5910	0.058*
C24	0.5846 (2)	0.3878 (2)	0.4090 (3)	0.0387 (9)
H24A	0.5912	0.3313	0.4384	0.046*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0289 (5)	0.0299 (5)	0.0332 (5)	−0.0017 (4)	0.0037 (4)	0.0001 (4)
S2	0.0277 (5)	0.0332 (6)	0.0339 (5)	−0.0006 (4)	0.0049 (4)	−0.0033 (4)
O1	0.0299 (13)	0.0412 (15)	0.0465 (13)	−0.0085 (11)	0.0112 (11)	0.0047 (11)
O2	0.0341 (13)	0.0312 (14)	0.0415 (13)	0.0064 (11)	0.0029 (10)	−0.0002 (11)
O3	0.0299 (14)	0.0460 (16)	0.0406 (13)	−0.0055 (12)	0.0090 (10)	−0.0136 (11)
O4	0.0412 (14)	0.0584 (17)	0.0304 (12)	−0.0075 (13)	0.0112 (10)	−0.0024 (11)
O5	0.0329 (13)	0.0313 (15)	0.0652 (15)	0.0065 (12)	0.0048 (11)	−0.0052 (12)
F1	0.0491 (13)	0.0766 (17)	0.0446 (12)	0.0151 (12)	0.0096 (10)	0.0244 (11)
F2	0.0787 (17)	0.090 (2)	0.0900 (17)	−0.0365 (15)	0.0284 (14)	−0.0590 (16)
C1	0.038 (2)	0.041 (2)	0.0298 (19)	0.0054 (18)	0.0020 (17)	0.0033 (16)
C2	0.038 (2)	0.048 (2)	0.039 (2)	0.0067 (19)	0.0164 (16)	0.0064 (18)
C3	0.0279 (19)	0.034 (2)	0.0409 (19)	0.0040 (16)	0.0087 (16)	0.0009 (16)
C4	0.0277 (19)	0.028 (2)	0.0284 (17)	−0.0005 (16)	0.0024 (15)	−0.0021 (14)
C5	0.0267 (19)	0.042 (2)	0.0367 (19)	−0.0009 (17)	0.0092 (15)	−0.0020 (17)
C6	0.0261 (19)	0.050 (2)	0.040 (2)	0.0070 (18)	0.0027 (16)	0.0015 (18)
C7	0.0252 (19)	0.027 (2)	0.0269 (16)	0.0006 (15)	0.0033 (14)	0.0038 (14)

C8	0.0274 (19)	0.038 (2)	0.0286 (17)	0.0045 (16)	0.0086 (14)	−0.0002 (16)
C9	0.0193 (17)	0.045 (2)	0.0304 (17)	−0.0031 (17)	0.0051 (14)	−0.0017 (17)
C10	0.028 (2)	0.030 (2)	0.0238 (16)	−0.0020 (16)	0.0036 (14)	−0.0003 (15)
C11	0.0254 (19)	0.038 (2)	0.0302 (17)	0.0028 (16)	0.0088 (14)	−0.0003 (16)
C12	0.0228 (18)	0.037 (2)	0.0338 (18)	−0.0001 (17)	0.0040 (15)	0.0034 (16)
C13	0.0248 (19)	0.041 (2)	0.0265 (17)	−0.0019 (17)	0.0059 (15)	−0.0082 (16)
C14	0.030 (2)	0.042 (2)	0.0357 (18)	0.0065 (17)	0.0017 (15)	0.0091 (17)
C15	0.033 (2)	0.038 (2)	0.041 (2)	−0.0004 (18)	0.0082 (16)	0.0093 (17)
C16	0.0307 (19)	0.023 (2)	0.0245 (16)	0.0006 (15)	0.0014 (14)	−0.0026 (15)
C17	0.038 (2)	0.030 (2)	0.0303 (17)	0.0003 (17)	0.0019 (15)	0.0025 (16)
C18	0.037 (2)	0.031 (2)	0.0350 (19)	−0.0043 (17)	0.0109 (16)	0.0034 (16)
C19	0.0231 (17)	0.030 (2)	0.0334 (18)	−0.0038 (16)	0.0092 (14)	−0.0007 (16)
C20	0.043 (2)	0.037 (2)	0.0411 (19)	−0.0020 (19)	0.0153 (17)	0.0013 (18)
C21	0.053 (2)	0.034 (2)	0.064 (3)	−0.010 (2)	0.026 (2)	−0.005 (2)
C22	0.038 (2)	0.056 (3)	0.059 (3)	−0.016 (2)	0.020 (2)	−0.033 (2)
C23	0.036 (2)	0.071 (3)	0.035 (2)	0.000 (2)	0.0025 (16)	−0.011 (2)
C24	0.035 (2)	0.046 (2)	0.0335 (19)	0.0066 (18)	0.0026 (16)	0.0006 (17)

Geometric parameters (Å, °)

S1—O1	1.436 (2)	C9—C10	1.382 (4)
S1—O2	1.439 (2)	C9—H9A	0.9500
S1—C7	1.754 (3)	C10—C11	1.387 (4)
S1—C4	1.772 (3)	C11—C12	1.370 (4)
S2—O5	1.432 (2)	C11—H11A	0.9500
S2—O4	1.440 (2)	C12—H12A	0.9500
S2—C19	1.759 (3)	C13—C18	1.372 (4)
S2—C16	1.762 (3)	C13—C14	1.376 (5)
O3—C10	1.381 (4)	C14—C15	1.381 (4)
O3—C13	1.397 (4)	C14—H14A	0.9500
F1—C1	1.359 (4)	C15—C16	1.384 (4)
F2—C22	1.363 (4)	C15—H15A	0.9500
C1—C6	1.362 (4)	C16—C17	1.384 (4)
C1—C2	1.365 (4)	C17—C18	1.382 (4)
C2—C3	1.383 (4)	C17—H17A	0.9500
C2—H2A	0.9500	C18—H18A	0.9500
C3—C4	1.380 (4)	C19—C20	1.381 (5)
C3—H3A	0.9500	C19—C24	1.387 (4)
C4—C5	1.384 (4)	C20—C21	1.374 (5)
C5—C6	1.390 (4)	C20—H20A	0.9500
C5—H5A	0.9500	C21—C22	1.353 (5)
C6—H6A	0.9500	C21—H21A	0.9500
C7—C8	1.390 (4)	C22—C23	1.372 (5)
C7—C12	1.391 (4)	C23—C24	1.371 (5)
C8—C9	1.379 (4)	C23—H23A	0.9500
C8—H8A	0.9500	C24—H24A	0.9500
O1—S1—O2	119.54 (14)	C12—C11—C10	119.6 (3)
O1—S1—C7	109.04 (14)	C12—C11—H11A	120.2
O2—S1—C7	107.93 (13)	C10—C11—H11A	120.2

O1—S1—C4	107.54 (14)	C11—C12—C7	119.9 (3)
O2—S1—C4	107.03 (14)	C11—C12—H12A	120.1
C7—S1—C4	104.80 (14)	C7—C12—H12A	120.1
O5—S2—O4	119.39 (15)	C18—C13—C14	121.6 (3)
O5—S2—C19	107.87 (14)	C18—C13—O3	119.6 (3)
O4—S2—C19	107.08 (15)	C14—C13—O3	118.8 (3)
O5—S2—C16	107.39 (14)	C13—C14—C15	119.2 (3)
O4—S2—C16	107.11 (13)	C13—C14—H14A	120.4
C19—S2—C16	107.50 (14)	C15—C14—H14A	120.4
C10—O3—C13	117.9 (2)	C14—C15—C16	119.7 (3)
F1—C1—C6	118.7 (3)	C14—C15—H15A	120.1
F1—C1—C2	117.5 (3)	C16—C15—H15A	120.1
C6—C1—C2	123.8 (3)	C17—C16—C15	120.3 (3)
C1—C2—C3	118.0 (3)	C17—C16—S2	119.6 (2)
C1—C2—H2A	121.0	C15—C16—S2	119.9 (2)
C3—C2—H2A	121.0	C18—C17—C16	119.8 (3)
C4—C3—C2	120.0 (3)	C18—C17—H17A	120.1
C4—C3—H3A	120.0	C16—C17—H17A	120.1
C2—C3—H3A	120.0	C13—C18—C17	119.3 (3)
C3—C4—C5	120.7 (3)	C13—C18—H18A	120.4
C3—C4—S1	119.4 (2)	C17—C18—H18A	120.4
C5—C4—S1	119.9 (2)	C20—C19—C24	120.3 (3)
C4—C5—C6	119.5 (3)	C20—C19—S2	119.1 (2)
C4—C5—H5A	120.2	C24—C19—S2	120.5 (3)
C6—C5—H5A	120.2	C21—C20—C19	120.0 (3)
C1—C6—C5	118.1 (3)	C21—C20—H20A	120.0
C1—C6—H6A	121.0	C19—C20—H20A	120.0
C5—C6—H6A	121.0	C22—C21—C20	118.1 (4)
C8—C7—C12	120.2 (3)	C22—C21—H21A	120.9
C8—C7—S1	119.7 (2)	C20—C21—H21A	120.9
C12—C7—S1	120.1 (2)	C21—C22—F2	118.7 (4)
C9—C8—C7	120.0 (3)	C21—C22—C23	123.8 (3)
C9—C8—H8A	120.0	F2—C22—C23	117.5 (4)
C7—C8—H8A	120.0	C24—C23—C22	117.9 (3)
C8—C9—C10	119.2 (3)	C24—C23—H23A	121.0
C8—C9—H9A	120.4	C22—C23—H23A	121.0
C10—C9—H9A	120.4	C23—C24—C19	119.8 (3)
O3—C10—C9	123.8 (3)	C23—C24—H24A	120.1
O3—C10—C11	115.0 (3)	C19—C24—H24A	120.1
C9—C10—C11	121.2 (3)		
F1—C1—C2—C3	178.9 (3)	C10—O3—C13—C18	−85.5 (3)
C6—C1—C2—C3	−0.9 (5)	C10—O3—C13—C14	95.6 (4)
C1—C2—C3—C4	0.3 (5)	C18—C13—C14—C15	3.1 (5)
C2—C3—C4—C5	0.5 (5)	O3—C13—C14—C15	−178.0 (3)
C2—C3—C4—S1	178.7 (3)	C13—C14—C15—C16	−0.8 (5)
O1—S1—C4—C3	−159.3 (3)	C14—C15—C16—C17	−2.5 (5)
O2—S1—C4—C3	−29.7 (3)	C14—C15—C16—S2	172.6 (2)
C7—S1—C4—C3	84.8 (3)	O5—S2—C16—C17	19.8 (3)
O1—S1—C4—C5	18.9 (3)	O4—S2—C16—C17	149.1 (2)

O2—S1—C4—C5	148.6 (3)	C19—S2—C16—C17	−96.1 (3)
C7—S1—C4—C5	−97.0 (3)	O5—S2—C16—C15	−155.3 (2)
C3—C4—C5—C6	−0.8 (5)	O4—S2—C16—C15	−26.0 (3)
S1—C4—C5—C6	−179.1 (2)	C19—S2—C16—C15	88.8 (3)
F1—C1—C6—C5	−179.2 (3)	C15—C16—C17—C18	3.5 (5)
C2—C1—C6—C5	0.5 (5)	S2—C16—C17—C18	−171.6 (2)
C4—C5—C6—C1	0.4 (5)	C14—C13—C18—C17	−2.1 (5)
O1—S1—C7—C8	152.6 (2)	O3—C13—C18—C17	179.0 (3)
O2—S1—C7—C8	21.3 (3)	C16—C17—C18—C13	−1.3 (5)
C4—S1—C7—C8	−92.5 (3)	O5—S2—C19—C20	160.3 (2)
O1—S1—C7—C12	−29.3 (3)	O4—S2—C19—C20	30.7 (3)
O2—S1—C7—C12	−160.6 (2)	C16—S2—C19—C20	−84.1 (3)
C4—S1—C7—C12	85.6 (3)	O5—S2—C19—C24	−17.1 (3)
C12—C7—C8—C9	−1.2 (4)	O4—S2—C19—C24	−146.8 (2)
S1—C7—C8—C9	176.9 (2)	C16—S2—C19—C24	98.4 (3)
C7—C8—C9—C10	0.5 (5)	C24—C19—C20—C21	0.7 (5)
C13—O3—C10—C9	5.3 (4)	S2—C19—C20—C21	−176.8 (3)
C13—O3—C10—C11	−174.0 (3)	C19—C20—C21—C22	1.3 (5)
C8—C9—C10—O3	−179.0 (3)	C20—C21—C22—F2	178.1 (3)
C8—C9—C10—C11	0.2 (5)	C20—C21—C22—C23	−2.6 (6)
O3—C10—C11—C12	179.1 (3)	C21—C22—C23—C24	1.7 (6)
C9—C10—C11—C12	−0.2 (5)	F2—C22—C23—C24	−179.0 (3)
C10—C11—C12—C7	−0.6 (5)	C22—C23—C24—C19	0.4 (5)
C8—C7—C12—C11	1.3 (4)	C20—C19—C24—C23	−1.6 (5)
S1—C7—C12—C11	−176.9 (2)	S2—C19—C24—C23	175.8 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2A···O2^{i}	0.95	2.55	3.206 (4)	126
C6—H6A···O5^{ii}	0.95	2.53	3.337 (4)	143
C14—H14A···O2^{iii}	0.95	2.47	3.361 (4)	157
C17—H17A···O4^{iv}	0.95	2.60	3.529 (4)	168
C11—H11A···F1^{v}	0.95	2.67	3.396 (4)	134
C23—H23A···F1^{vi}	0.95	2.65	3.373 (5)	133
C11—H11A···Cg1^{iv}	0.95	2.97	3.541 (3)	120

Symmetry codes: (i) −*x*, −*y*, −*z*−1; (ii) *x*−1, *y*, *z*−1; (iii) −*x*, *y*+1/2, −*z*−1/2; (iv) *x*, −*y*+1/2, *z*+1/2; (v) *x*, *y*, *z*+1; (vi) *x*+1, −*y*+1/2, *z*+3/2.

Fig. 1

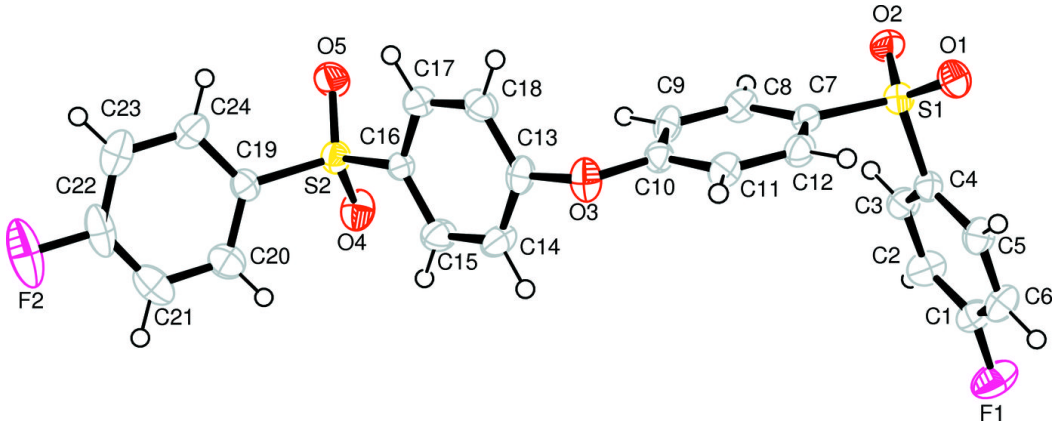
O2
O1
O5
C17
C18
C9
C8
C7
S1
C23
C24
C16
C13
C19
S2
C22
O3
C10
C11
C12
C4
C3
O4
C5
C2
C20
C15
C14
C6
F2
C21
C1
F1

Fig. 2