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(2-Methoxy-5-methylphenyl)(4-methoxy-2-methylphenyl)iodonium trifluoroacetate

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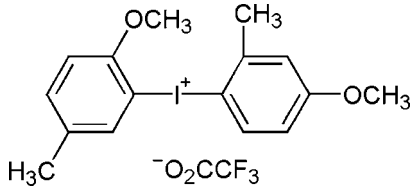
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.015 Å; disorder in solvent or counterion; R factor = 0.056; wR factor = 0.169; data-to-parameter ratio = 12.8.

The asymmetric unit of the title compound, $C_{16}H_{18}IO_2^+\cdot CF_3CO_2^-$, comprises an iodonium cation and a trifluoroacetate anion, in which the F atoms are disordered over two postions of equal occupancy. The benzene rings are inclined at 87.76 (5)° to one another. Extremely short intermolecular I···O contacts [2.807 (9) and 3.019 (13) Å] occur, due to strong electrostatic interactions between the I atom and two adjacent trifluoroacetate counter-ions.

Related literature

For related literature, see: Shah *et al.* (1997, 1998); Li & Jiang (2007).



Experimental

Crystal data

$C_{16}H_{18}IO_2^+\cdot C_2F_3O_2^-$
M_r = 482.22
Triclinic, $P\overline{1}$
a = 8.211 (4) Å
b = 11.182 (6) Å
c = 12.200 (6) Å
α = 93.690 (8)°
β = 107.874 (7)°
γ = 109.841 (8)°
V = 984.9 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.67 mm^{-1}
T = 294 (2) K
0.20 × 0.18 × 0.14 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.731, T_{max} = 0.800
4842 measured reflections
3425 independent reflections
2356 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.169
S = 1.01
3425 reflections
267 parameters
72 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.78 e Å^{-3}

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2492).

References

Bruker (1997). *SMART* (Version 5.611), *SAINT* (Version 5.01) and *SHELXTL* (Version 6.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Li, H. & Jiang, S. (2007). *Acta Cryst.* E**63**, o83–o85.
Shah, A., Pike, V. W. & Widdowson, D. A. (1997). *J. Chem. Soc. Perkin Trans. 1*, pp. 2463–2465.
Shah, A., Pike, V. W. & Widdowson, D. A. (1998). *J. Chem. Soc. Perkin Trans. 1*, pp. 2043–2046.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

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supplementary materials

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(2-Methoxy-5-methylphenyl)(4-methoxy-2-methylphenyl)iodonium trifluoroacetate

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Comment

Diaryliodonium salts are useful in organic synthesis for arylation of organic and inorganic bases (Shah *et al.*, 1997; Shah *et al.*, 1998). The title compound, (I), (Fig. 1), is an important representative of such reagents. The iodine atom lies almost in the plane of both attached benzene rings with r.m.s. deviations of 0.022 (3) Å and 0.015 (3) Å from the C1—C6 and C9—C14 mean planes respectively. These rings are nearly orthogonal with a dihedral angle between them of 87.76 (5) °.

Each iodine atom interacts with two O atoms from adjacent trifloroacetate anions. Inversion symmetry then generates cyclic units (Fig. 2). Similar interactions have been observed previously in iodonium salts (Li & Jiang, 2007). The distances I1—O3^{i} and I1—O3^{ii} (i = $x-1, y+1, z$; ii = $1-x, 1-y, -z$) in (I) are 3.019 (13) and 2.807 (9) Å, respectively.

Experimental

Sodium perborate tetrahydrate (35.39 g, 230 mmol) was added in batches to a stirred mixture of 2-iodo-4-methylanisole (5.71 g, 23 mmol) in acetic acid (100 ml) and acetic anhydride (50 ml) at 318 K. The suspension was stirred for 4.5 h at 318 K, diluted with 600 ml of water and extracted three times with dichloromethane. The organic extracts were dried with sodium sulfate, the solvent removed in vacuum and the residue crystallized from diethyl ether to obtain 2-methoxy-5-methylbis(acetoxy)iodobenzene.

Trifluoromethanesulfonic acid (0.63 ml, 8.2 mmol) was added dropwise to a stirred suspension of this product (1.5 g, 4.1 mmol) in dichloromethane (50 ml) at 263 K under nitrogen. The mixture was stirred for 30 min at 263 K, then at room temperature for a further 1.5 h, cooled to 263 K and 3-methylanisole (0.50 g, 4.1 mmol) added dropwise *via* syringe. The mixture was stirred at 263 K for 1 h and then at room temperature overnight, solvent was removed in vacuum and the residue crystallized from diethyl ether. Crystals suitable for X-ray analysis were obtained by slow evaporation in dichloromethane solution.

Refinement

The fluorine atoms in the CF_3 group were found to be disordered over two positions. Their occupancy factors refined to 0.512 (18) and 0.488 (18) respectively. The C—F distance was restrained to 1.37 (1) Å.

All the H atoms were positioned geometrically (C—H = 0.93–0.96 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

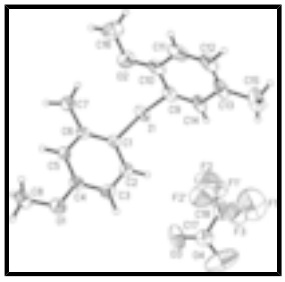

Fig. 1. The asymmetric unit of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii. Open bonds connect atoms of the minor disorder component of the CF_3 group.

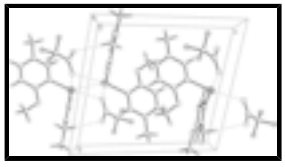

Fig. 2. The crystal packing for (I). Dashed lines represent intermolecular I···O interactions.

(2-Methoxy-5-methylphenyl)(4-methoxy-2-methylphenyl)iodonium trifluoroacetate

Crystal data

$C_{16}H_{18}IO_2^+ \cdot C_2F_3O_2^-$	$Z = 2$
$M_r = 482.22$	$F_{000} = 476$
Triclinic, $P\overline{1}$	$D_x = 1.626$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.211$ (4) Å	Cell parameters from 2102 reflections
$b = 11.182$ (6) Å	$\theta = 2.4$–24.9º
$c = 12.200$ (6) Å	$\mu = 1.67$ mm^{-1}
$\alpha = 93.690$ (8)º	$T = 294$ (2) K
$\beta = 107.874$ (7)º	Block, colourless
$\gamma = 109.841$ (8)º	0.20 × 0.18 × 0.14 mm
$V = 984.9$ (8) Å^3	

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	3425 independent reflections
Radiation source: fine-focus sealed tube	2356 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.026$
$T = 294$(2) K	$\theta_{max} = 25.0$º
ω scans	$\theta_{min} = 1.8$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -9 \rightarrow 8$
$T_{min} = 0.731$, $T_{max} = 0.800$	$k = -13 \rightarrow 13$
4842 measured reflections	$l = -8 \rightarrow 14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.056$	H-atom parameters constrained
$wR(F^2) = 0.169$	$w = 1/[\sigma^2(F_o^2) + (0.0996P)^2 + 1.2747P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.004$
3425 reflections	$\Delta\rho_{max} = 1.20$ e Å^{-3}
267 parameters	$\Delta\rho_{min} = -0.78$ e Å^{-3}
72 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

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 $F^2 > 2\text{sigma}(F^2)$ 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}	Occ. (<1)
I1	0.19140 (9)	0.97059 (6)	0.12590 (4)	0.0615 (3)	
O1	0.6312 (9)	0.6100 (7)	0.1571 (7)	0.082 (2)	
O2	0.1034 (10)	0.8681 (8)	0.3388 (6)	0.079 (2)	
C1	0.3292 (11)	0.8419 (7)	0.1341 (6)	0.0426 (18)	
C2	0.5130 (12)	0.8923 (9)	0.1423 (8)	0.057 (2)	
H2	0.5706	0.9802	0.1440	0.068*	
C3	0.6100 (12)	0.8126 (10)	0.1480 (9)	0.065 (2)	
H3	0.7324	0.8454	0.1520	0.078*	
C4	0.5232 (11)	0.6840 (9)	0.1477 (8)	0.054 (2)	
C5	0.3393 (11)	0.6320 (8)	0.1396 (7)	0.0465 (18)	
H5	0.2836	0.5442	0.1388	0.056*	
C6	0.2382 (10)	0.7105 (8)	0.1327 (6)	0.0452 (19)	
C7	0.0350 (12)	0.6463 (10)	0.1190 (10)	0.074 (3)	
H7A	0.0033	0.5549	0.1161	0.111*	
H7B	−0.0404	0.6607	0.0477	0.111*	
H7C	0.0143	0.6827	0.1844	0.111*	
C8	0.5516 (17)	0.4762 (11)	0.1592 (13)	0.096 (4)	

H8A	0.5154	0.4663	0.2269	0.144*	
H8B	0.6405	0.4374	0.1627	0.144*	
H8C	0.4450	0.4346	0.0895	0.144*	
C9	0.3077 (12)	1.0572 (9)	0.3044 (7)	0.055 (2)	
C10	0.2357 (14)	0.9876 (11)	0.3836 (7)	0.063 (2)	
C11	0.3145 (17)	1.0517 (13)	0.5011 (8)	0.080 (3)	
H11	0.2757	1.0099	0.5573	0.096*	
C12	0.4429 (16)	1.1706 (13)	0.5338 (8)	0.079 (3)	
H12	0.4872	1.2099	0.6122	0.095*	
C13	0.5142 (16)	1.2393 (12)	0.4585 (10)	0.084 (4)	
C14	0.4398 (14)	1.1769 (10)	0.3386 (9)	0.066 (3)	
H14	0.4828	1.2191	0.2838	0.079*	
C15	0.658 (2)	1.3747 (12)	0.4951 (13)	0.119 (5)	
H15A	0.6070	1.4332	0.5185	0.179*	
H15B	0.6967	1.3997	0.4304	0.179*	
H15C	0.7627	1.3777	0.5597	0.179*	
C16	0.0146 (19)	0.8018 (14)	0.4130 (12)	0.107 (4)	
H16A	0.1041	0.7881	0.4775	0.161*	
H16B	−0.0786	0.7198	0.3691	0.161*	
H16C	−0.0418	0.8528	0.4423	0.161*	
F1	0.964 (3)	0.3874 (13)	0.2500 (18)	0.143 (8)	0.488 (18)
F2	0.813 (2)	0.208 (2)	0.282 (2)	0.167 (9)	0.488 (18)
F3	1.101 (2)	0.2949 (18)	0.3656 (11)	0.124 (7)	0.488 (18)
F1'	0.794 (2)	0.267 (2)	0.2015 (18)	0.157 (9)	0.512 (18)
F2'	0.924 (3)	0.1712 (17)	0.3198 (16)	0.153 (8)	0.512 (18)
F3'	1.052 (4)	0.3757 (18)	0.336 (2)	0.269 (18)	0.512 (18)
C17	1.0118 (16)	0.2125 (12)	0.1657 (9)	0.068 (3)	
C18	0.9657 (16)	0.2663 (10)	0.2565 (10)	0.110 (4)	
O3	0.9273 (16)	0.1057 (9)	0.1183 (8)	0.115 (3)	
O4	1.1470 (18)	0.2865 (18)	0.1514 (14)	0.210 (8)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.0862 (5)	0.0779 (5)	0.0292 (3)	0.0555 (4)	0.0053 (3)	0.0064 (2)
O1	0.063 (4)	0.072 (5)	0.125 (7)	0.042 (4)	0.033 (4)	0.019 (4)
O2	0.085 (5)	0.092 (5)	0.046 (4)	0.022 (4)	0.016 (4)	0.010 (4)
C1	0.054 (5)	0.045 (5)	0.032 (4)	0.027 (4)	0.010 (3)	0.008 (3)
C2	0.057 (6)	0.054 (5)	0.059 (5)	0.019 (4)	0.022 (4)	0.008 (4)
C3	0.046 (5)	0.069 (7)	0.082 (7)	0.020 (5)	0.027 (5)	0.014 (5)
C4	0.045 (5)	0.060 (6)	0.059 (5)	0.027 (4)	0.013 (4)	0.009 (4)
C5	0.050 (5)	0.048 (5)	0.042 (4)	0.021 (4)	0.014 (4)	0.006 (4)
C6	0.038 (4)	0.065 (6)	0.033 (4)	0.025 (4)	0.008 (3)	0.003 (3)
C7	0.048 (5)	0.071 (7)	0.091 (7)	0.018 (5)	0.018 (5)	−0.007 (5)
C8	0.108 (9)	0.078 (8)	0.138 (12)	0.064 (7)	0.056 (9)	0.035 (7)
C9	0.069 (6)	0.065 (6)	0.033 (4)	0.046 (5)	0.001 (4)	0.008 (4)
C10	0.075 (6)	0.092 (8)	0.034 (4)	0.053 (6)	0.012 (4)	0.009 (5)
C11	0.100 (8)	0.122 (10)	0.039 (5)	0.072 (8)	0.019 (6)	0.014 (6)

C12	0.096 (8)	0.105 (9)	0.027 (5)	0.050 (7)	0.001 (5)	−0.011 (5)
C13	0.089 (7)	0.087 (8)	0.055 (6)	0.048 (7)	−0.013 (6)	−0.026 (6)
C14	0.081 (7)	0.061 (6)	0.056 (5)	0.043 (6)	0.007 (5)	0.002 (5)
C15	0.131 (11)	0.078 (9)	0.116 (11)	0.037 (8)	0.009 (9)	−0.015 (8)
C16	0.104 (9)	0.138 (12)	0.087 (9)	0.040 (9)	0.045 (8)	0.032 (9)
F1	0.169 (12)	0.106 (10)	0.157 (12)	0.084 (9)	0.029 (8)	0.005 (7)
F2	0.150 (11)	0.206 (14)	0.164 (13)	0.053 (8)	0.104 (10)	0.006 (8)
F3	0.142 (10)	0.134 (11)	0.087 (9)	0.056 (8)	0.029 (7)	0.000 (7)
F1'	0.156 (11)	0.165 (12)	0.189 (13)	0.087 (9)	0.081 (9)	0.030 (8)
F2'	0.177 (12)	0.185 (12)	0.108 (10)	0.052 (8)	0.078 (9)	0.050 (8)
F3'	0.28 (2)	0.25 (2)	0.27 (2)	0.110 (12)	0.083 (12)	0.029 (10)
C17	0.070 (7)	0.085 (8)	0.056 (6)	0.040 (6)	0.016 (5)	0.032 (6)
C18	0.140 (13)	0.081 (9)	0.095 (10)	0.028 (9)	0.044 (10)	−0.008 (7)
O3	0.175 (9)	0.084 (6)	0.072 (5)	0.055 (6)	0.022 (6)	−0.008 (5)
O4	0.131 (9)	0.31 (2)	0.211 (16)	0.068 (12)	0.091 (11)	0.154 (15)

Geometric parameters (Å, °)

I1—C1	2.101 (7)	C10—C11	1.404 (13)
I1—C9	2.102 (8)	C11—C12	1.327 (16)
O1—C4	1.390 (10)	C11—H11	0.9300
O1—C8	1.420 (13)	C12—C13	1.376 (17)
O2—C10	1.349 (13)	C12—H12	0.9300
O2—C16	1.423 (14)	C13—C14	1.426 (14)
C1—C2	1.389 (12)	C13—C15	1.504 (18)
C1—C6	1.400 (11)	C14—H14	0.9300
C2—C3	1.375 (12)	C15—H15A	0.9600
C2—H2	0.9300	C15—H15B	0.9600
C3—C4	1.371 (13)	C15—H15C	0.9600
C3—H3	0.9300	C16—H16A	0.9600
C4—C5	1.391 (12)	C16—H16B	0.9600
C5—C6	1.388 (11)	C16—H16C	0.9600
C5—H5	0.9300	F1—C18	1.365 (8)
C6—C7	1.526 (12)	F2—C18	1.343 (8)
C7—H7A	0.9600	F3—C18	1.380 (8)
C7—H7B	0.9600	F1'—C18	1.367 (8)
C7—H7C	0.9600	F2'—C18	1.366 (8)
C8—H8A	0.9600	F3'—C18	1.331 (9)
C8—H8B	0.9600	C17—O3	1.159 (13)
C8—H8C	0.9600	C17—O4	1.209 (15)
C9—C14	1.344 (14)	C17—C18	1.435 (15)
C9—C10	1.422 (14)		
C1—I1—C9	97.7 (3)	C13—C12—H12	118.0
C4—O1—C8	118.9 (7)	C12—C13—C14	116.3 (11)
C10—O2—C16	118.5 (9)	C12—C13—C15	124.0 (11)
C2—C1—C6	121.7 (7)	C14—C13—C15	119.7 (13)
C2—C1—I1	117.6 (6)	C9—C14—C13	120.1 (11)
C6—C1—I1	120.7 (5)	C9—C14—H14	119.9
C3—C2—C1	120.1 (8)	C13—C14—H14	119.9

C3—C2—H2	120.0	C13—C15—H15A	109.5
C1—C2—H2	120.0	C13—C15—H15B	109.5
C4—C3—C2	118.9 (8)	H15A—C15—H15B	109.5
C4—C3—H3	120.5	C13—C15—H15C	109.5
C2—C3—H3	120.5	H15A—C15—H15C	109.5
C3—C4—O1	115.7 (7)	H15B—C15—H15C	109.5
C3—C4—C5	121.7 (7)	O2—C16—H16A	109.5
O1—C4—C5	122.6 (8)	O2—C16—H16B	109.5
C6—C5—C4	120.4 (8)	H16A—C16—H16B	109.5
C6—C5—H5	119.8	O2—C16—H16C	109.5
C4—C5—H5	119.8	H16A—C16—H16C	109.5
C5—C6—C1	117.3 (7)	H16B—C16—H16C	109.5
C5—C6—C7	117.6 (8)	O3—C17—O4	126.6 (15)
C1—C6—C7	125.0 (7)	O3—C17—C18	120.0 (11)
C6—C7—H7A	109.5	O4—C17—C18	113.3 (14)
C6—C7—H7B	109.5	F3'—C18—F2	103 (2)
H7A—C7—H7B	109.5	F3'—C18—F1	48.9 (12)
C6—C7—H7C	109.5	F2—C18—F1	102.0 (12)
H7A—C7—H7C	109.5	F3'—C18—F2'	104.7 (13)
H7B—C7—H7C	109.5	F2—C18—F2'	48.5 (11)
O1—C8—H8A	109.5	F1—C18—F2'	139.8 (16)
O1—C8—H8B	109.5	F3'—C18—F1'	104.1 (12)
H8A—C8—H8B	109.5	F2—C18—F1'	53.2 (11)
O1—C8—H8C	109.5	F1—C18—F1'	66.5 (11)
H8A—C8—H8C	109.5	F2'—C18—F1'	100.2 (11)
H8B—C8—H8C	109.5	F3'—C18—F3	49.9 (12)
C14—C9—C10	122.7 (8)	F2—C18—F3	101.0 (11)
C14—C9—I1	119.4 (7)	F1—C18—F3	98.4 (10)
C10—C9—I1	117.8 (7)	F2'—C18—F3	68.2 (11)
O2—C10—C11	127.4 (10)	F1'—C18—F3	142.2 (15)
O2—C10—C9	117.2 (8)	F3'—C18—C17	132.8 (17)
C11—C10—C9	115.4 (11)	F2—C18—C17	124.5 (13)
C12—C11—C10	121.5 (11)	F1—C18—C17	114.4 (12)
C12—C11—H11	119.2	F2'—C18—C17	105.6 (12)
C10—C11—H11	119.2	F1'—C18—C17	105.1 (12)
C11—C12—C13	123.9 (9)	F3—C18—C17	112.7 (11)
C11—C12—H12	118.0		
C9—I1—C1—C2	−76.8 (7)	C14—C9—C10—C11	−1.1 (12)
C9—I1—C1—C6	102.4 (6)	I1—C9—C10—C11	−178.1 (6)
C6—C1—C2—C3	0.7 (13)	O2—C10—C11—C12	−179.2 (9)
I1—C1—C2—C3	180.0 (7)	C9—C10—C11—C12	2.1 (14)
C1—C2—C3—C4	−1.3 (14)	C10—C11—C12—C13	−2.3 (17)
C2—C3—C4—O1	−178.2 (9)	C11—C12—C13—C14	1.3 (16)
C2—C3—C4—C5	1.2 (15)	C11—C12—C13—C15	179.3 (11)
C8—O1—C4—C3	179.0 (10)	C10—C9—C14—C13	0.2 (13)
C8—O1—C4—C5	−0.4 (14)	I1—C9—C14—C13	177.2 (7)
C3—C4—C5—C6	−0.6 (13)	C12—C13—C14—C9	−0.2 (14)
O1—C4—C5—C6	178.7 (8)	C15—C13—C14—C9	−178.3 (10)
C4—C5—C6—C1	0.1 (11)	O3—C17—C18—F3'	168.4 (17)

C4—C5—C6—C7	177.6 (8)	O4—C17—C18—F3'	−8(2)
C2—C1—C6—C5	−0.1 (11)	O3—C17—C18—F2	−9.8 (19)
I1—C1—C6—C5	−179.4 (5)	O4—C17—C18—F2	173.7 (16)
C2—C1—C6—C7	−177.4 (9)	O3—C17—C18—F1	−135.9 (13)
I1—C1—C6—C7	3.4 (11)	O4—C17—C18—F1	47.6 (15)
C1—I1—C9—C14	104.3 (7)	O3—C17—C18—F2'	40.2 (15)
C1—I1—C9—C10	−78.6 (7)	O4—C17—C18—F2'	−136.3 (13)
C16—O2—C10—C11	8.0 (15)	O3—C17—C18—F1'	−65.2 (14)
C16—O2—C10—C9	−173.3 (9)	O4—C17—C18—F1'	118.3 (14)
C14—C9—C10—O2	−180.0 (8)	O3—C17—C18—F3	112.7 (13)
I1—C9—C10—O2	3.0 (10)	O4—C17—C18—F3	−63.8 (14)

Fig. 1

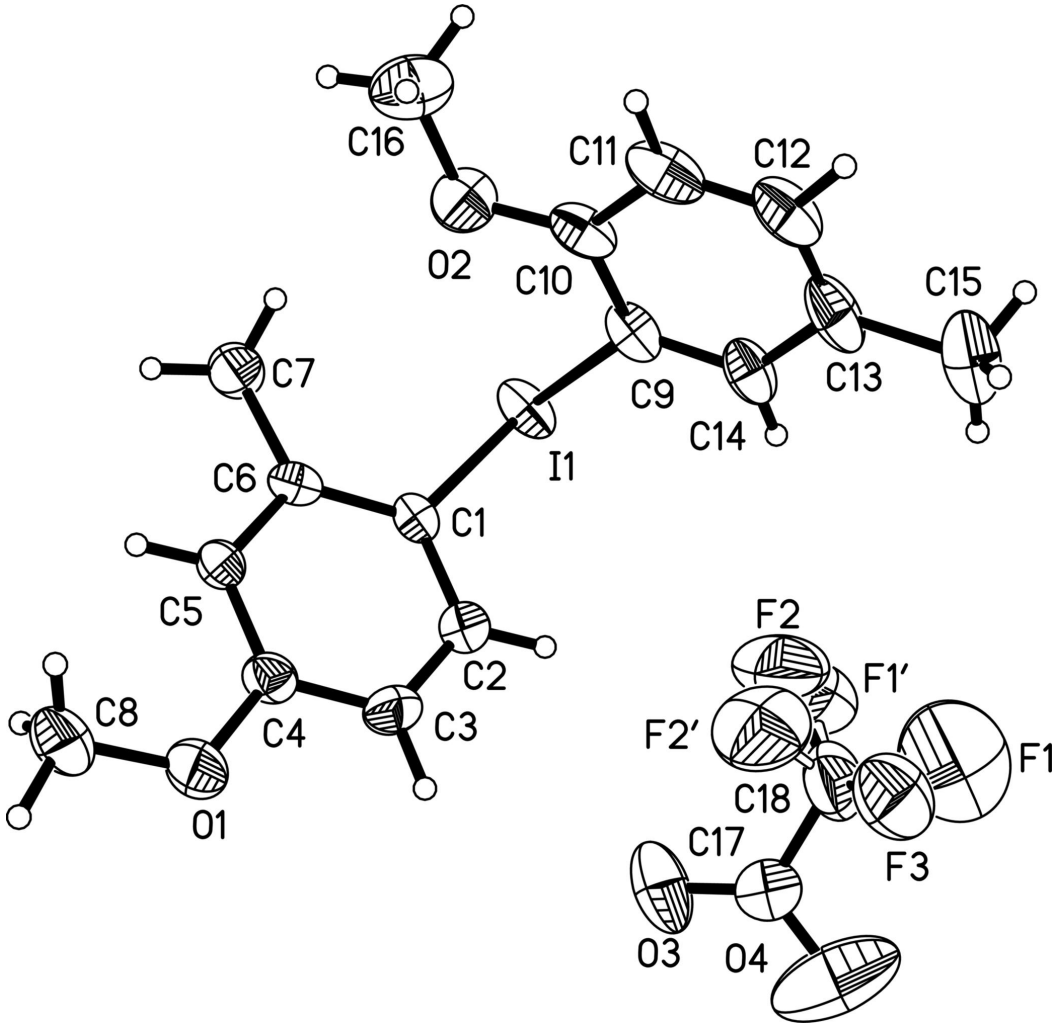
C16
C11
C12
O2
C10
C15
C7
C9
C13
C14
I1
C6
C1
C5
C2
C8
C4
C3
O1
F2
F1′
F2′
F1
C18
C17
F3
O3
O4

Fig. 2