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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.064
wR factor = 0.196
Data-to-parameter ratio = 12.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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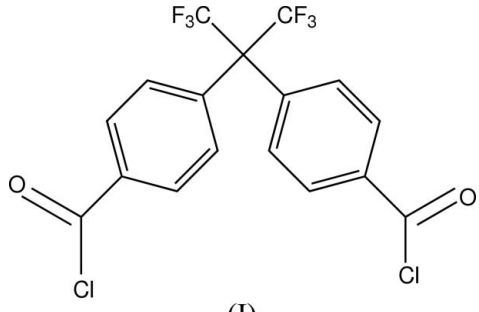
In the structure of the title molecule, $C_{17}H_8Cl_2F_6O_2$, the dihedral angle between the least-squares planes of the benzene rings is 66.31 (15)°. The CF_3 groups adopt an eclipsed conformation.

Comment

This paper reports a structural study of the title compound, (I) (Fig. 1). For an introduction and general discussion, see the preceding paper (Rodríguez de Barbarín *et al.*, 2006).



(I)

Experimental

Compound (I) was prepared as described in the preceding paper (Rodríguez de Barbarín *et al.*, 2006).

Crystal data

$C_{17}H_8Cl_2F_6O_2$
M_r = 429.13
Monoclinic, $C2/c$
a = 19.338 (9) Å
b = 12.299 (4) Å
c = 14.677 (4) Å
β = 98.12 (3)°
V = 3456 (2) Å^3
Z = 8
D_x = 1.650 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.45 mm^{-1}
T = 298 (1) K
Needle, colourless
0.60 × 0.20 × 0.18 mm

Data collection

Bruker $P4$ diffractometer
ω scans
Absorption correction: none
3727 measured reflections
3122 independent reflections
1830 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 25.4°
3 standard reflections
every 97 reflections
intensity decay: 6.4%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.196
S = 1.05
3122 reflections
244 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0714P)^2 + 9.4954P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

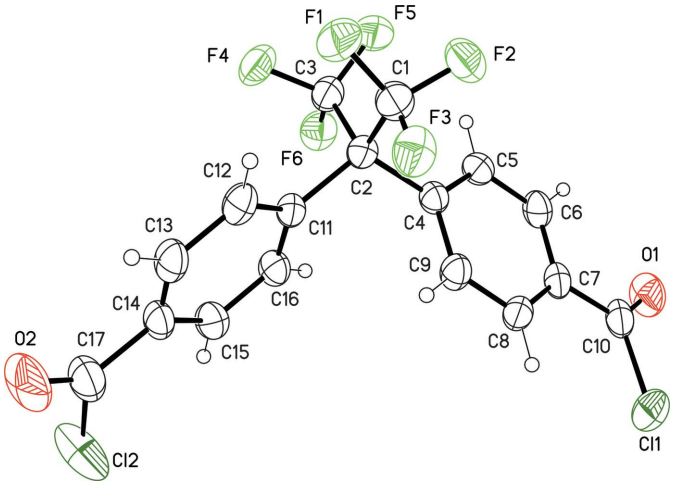


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

H atoms were placed in idealized positions (C—H = 0.93 Å) and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *XSCANS* (Siemens, 1996); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXTL-Plus* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL-Plus*; molecular graphics: *SHELXTL-Plus*; software used to prepare material for publication: *SHELXTL-Plus*.

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