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Recommended Citation

Rodríguez de Barbarín, C., Bernès, S., Macossay, J., & Cassidy, P. E. (2006). 4,4'-(1,1,1,3,3,3-Hexafluoropropane-2,2-diyl)bis(benzoyl chloride). *Acta Crystallographica Section E*, 62(8), o3602–o3603.
<https://doi.org/10.1107/S1600536806028236>

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Key indicators

Single-crystal X-ray study
 $T = 298$ K
 Mean $\sigma(\text{C}-\text{C}) = 0.006$ 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>.

4,4'-(1,1,1,3,3,3-Hexafluoropropane-2,2-diyl)-bis(benzoyl chloride)

In the structure of the title molecule, $\text{C}_{17}\text{H}_8\text{Cl}_2\text{F}_6\text{O}_2$, the dihedral angle between the least-squares planes of the benzene rings is 66.31 (15)°. The CF_3 groups adopt an eclipsed conformation.

Received 1 June 2006
 Accepted 20 July 2006

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).

Experimental

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

Crystal data

$\text{C}_{17}\text{H}_8\text{Cl}_2\text{F}_6\text{O}_2$
 $M_r = 429.13$
 Monoclinic, $C2/c$
 $a = 19.338$ (9) Å
 $b = 12.299$ (4) Å
 $c = 14.677$ (4) Å
 $\beta = 98.12$ (3)°
 $V = 3456$ (2) Å³

$Z = 8$
 $D_x = 1.650$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.45$ mm⁻¹
 $T = 298$ (1) K
 Needle, colourless
 $0.60 \times 0.20 \times 0.18$ mm

Data collection

Bruker *P4* diffractometer
 ω scans
 Absorption correction: none
 3727 measured reflections
 3122 independent reflections
 1830 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.031$
 $\theta_{\text{max}} = 25.4^\circ$
 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 $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.23$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.41$ 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 ($C-H = 0.93 \text{ \AA}$) 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*.

The authors thank Blanca Rodríguez (UANL) for experimental work.

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