Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-Fluorophenyl 4-{1,1,1,3,3,3-hexafluoro-2-[4-(4-fluorobenzoyl)phenyl]-2-propyl}-phenyl ketone

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Received 1 June 2006
Accepted 20 July 2006

Key indicators

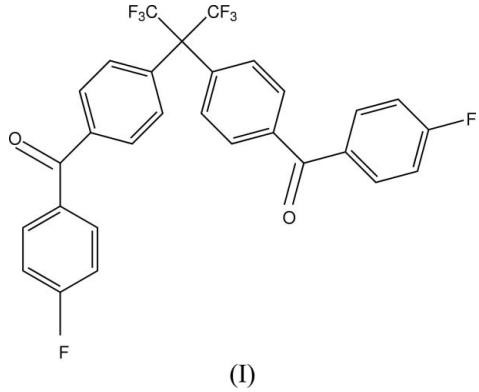
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.056
wR factor = 0.161
Data-to-parameter ratio = 12.5

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

In the title compound, $C_{29}H_{16}F_8O_2$, in spite of the symmetric substitution at the hexafluoropropane group, an unsymmetrical conformation is obtained for the fluorobenzoyl substituents. One substituent is oriented *syn* and the other *anti* to the central group.

Comment

As a part of our ongoing studies of poly(phenylene ether ketones) and hexafluoroisopropylidene-containing polymers (Cassidy *et al.*, 1989; Tullos *et al.*, 1990, 1991; Kane *et al.*, 1991; Bruma *et al.*, 1996), aiming at a systematic design of low dielectric polymers that could be used in the electronics industry, we report here the structure of the title compound, $C_{29}H_{16}F_8O_2$, (I).



(I)

In the title compound (Fig. 1) the dihedral angle between the least-squares planes of the benzene rings bonded to the central C2 atom is 79.16 (12)°, a larger value than that obtained in the precursor of (I), with a corresponding angle of 66.31 (15)° (Rodríguez de Barbarín *et al.*, 2006). The CF_3 groups adopt an eclipsed conformation in both compounds. In the title compound, the (4-fluorobenzoyl) substituents of both benzene rings have dihedral angles of 50.87 (15) (planes C4–C9 and C11–C16) and 54.80 (12)° (planes C17–C22 and C24–C29), respectively. In spite of the symmetric substitution at C2, an unsymmetrical conformation is obtained for the fluorobenzoyl groups: one is oriented *syn* and the other *anti* relative to the $C(CF_3)_2$ central core. The conformation of (I) is reflected in the packing, based on a triple-helix supramolecular arrangement (Fig. 2). The polymeric material, if retaining the structural characteristics described above for (I), would support a higher dielectric strain, which might explain the low dielectric constant observed for the corresponding poly(phenylene ether ketone) polymer (Tullos *et al.*, 1991; St Clair *et al.*, 1994).

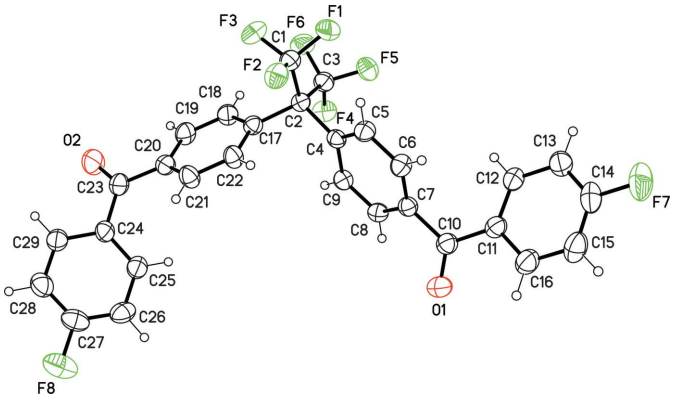


Figure 1
Molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level for non-H atoms.

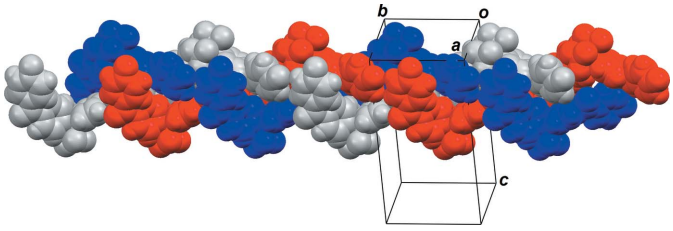


Figure 2
Part of the packing of (I) in a CPK space-filling representation, showing the supramolecular arrangement of the molecules along [010]. Each strand of the triple-helix framework is represented with a different colour.

Experimental

Compound (I) and its precursor were synthesized following the procedure outlined by St Clair *et al.* (1994). Single crystals for both compounds were obtained by slow evaporation of a methanol solution at 298 K.

Crystal data

$C_{29}H_{16}F_8O_2$
M_r = 548.42
Monoclinic, $P2_1/n$
a = 9.940 (2) Å
b = 11.202 (5) Å
c = 21.710 (9) Å
β = 90.68 (4)°
V = 2417.2 (16) Å^3
Z = 4
D_x = 1.507 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.14 mm^{-1}
T = 298 (1) K
Prism, colourless
0.60 × 0.16 × 0.04 mm

Data collection

Bruker $P4$ diffractometer
ω scans
5765 measured reflections
4396 independent reflections
2319 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 25.4°
3 standard reflections
every 97 reflections
intensity decay: <1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.161
S = 1.03
4396 reflections
353 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0533P)^2 + 1.9495P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Extinction correction: *SHELXTL-Plus*
Extinction coefficient: 0.0072 (10)

H atoms were placed in idealized positions (C—H = 0.93 Å) and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2 U_{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* and *MERCURY* (Version 1.4.1; Bruno *et al.*, 2002); software used to prepare material for publication: *SHELXTL-Plus*.

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

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